

## Supplementary Information

### Discovery of Nanomolar DCAF1 Small Molecule Ligands

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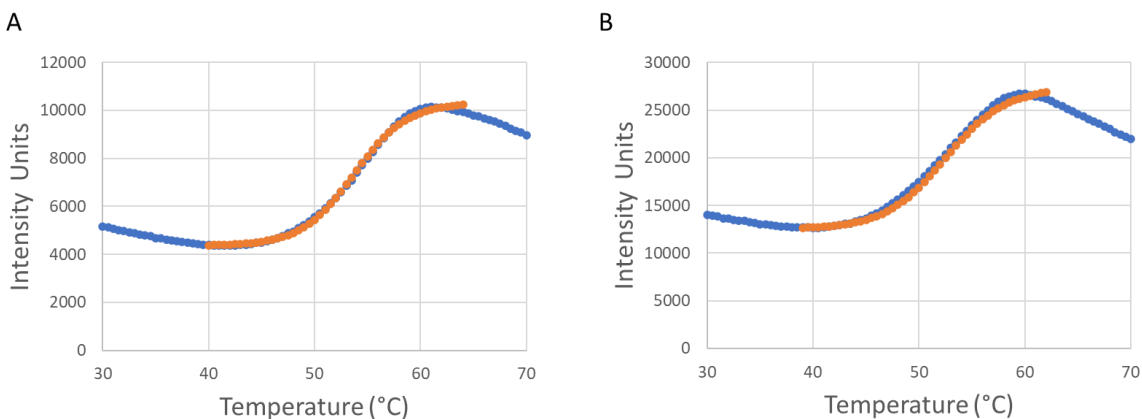
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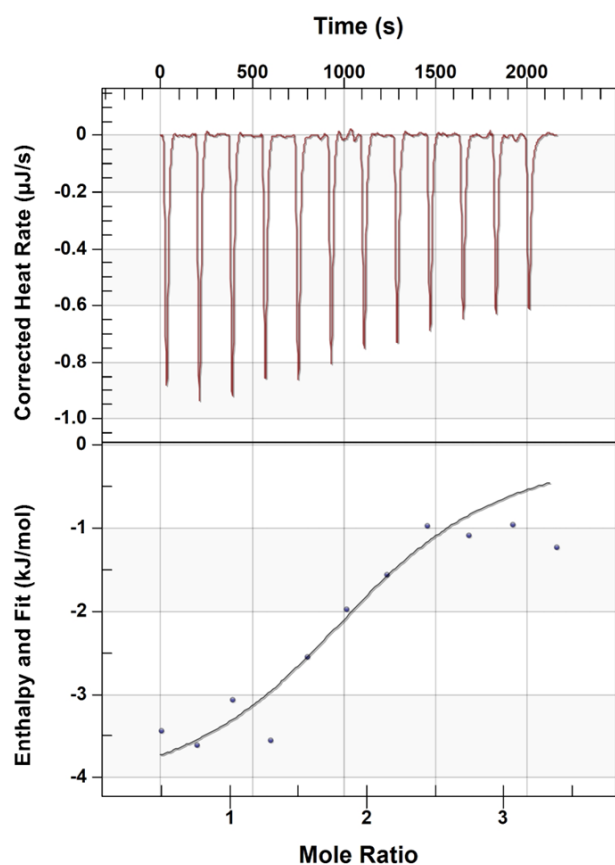
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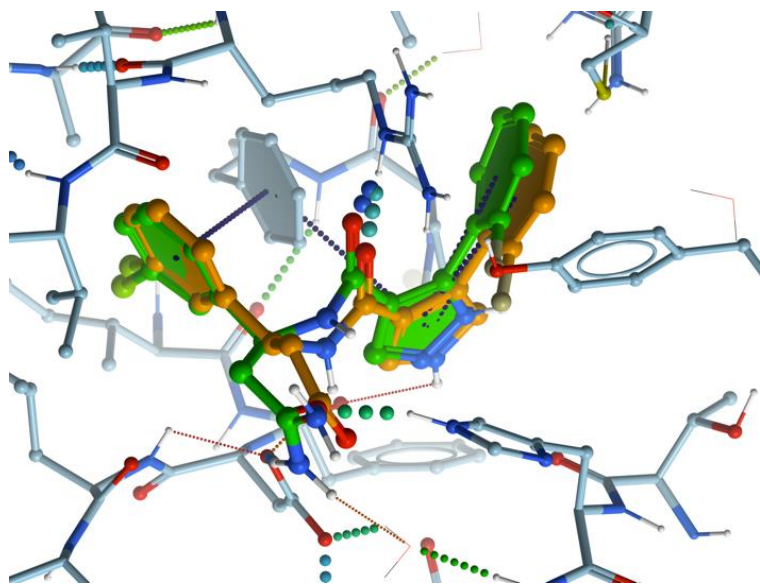
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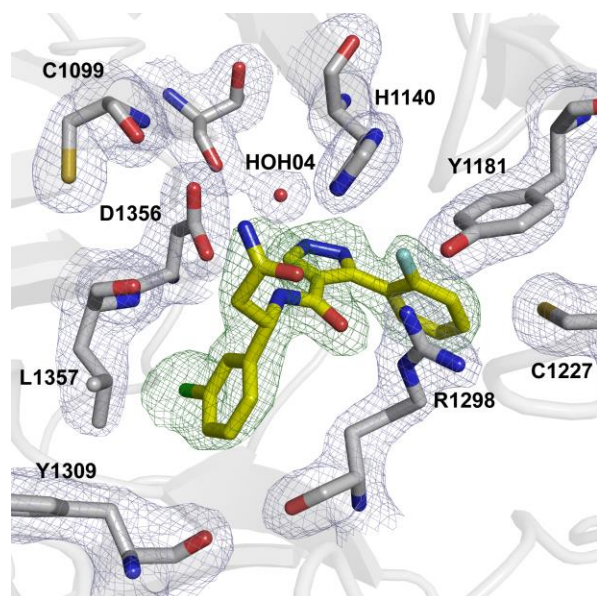
**Figure S1.** Melting curves of DCAF1 WDR domain. DCAF1 WDR domain showed amenability to differential scanning fluorimetry at two tested concentrations (A) 0.1 mg/mL and (B) 0.4 mg/mL. Both concentrations showed a transition with melting temperatures  $T_m$  of 53.7 °C and 52.0 °C, respectively.



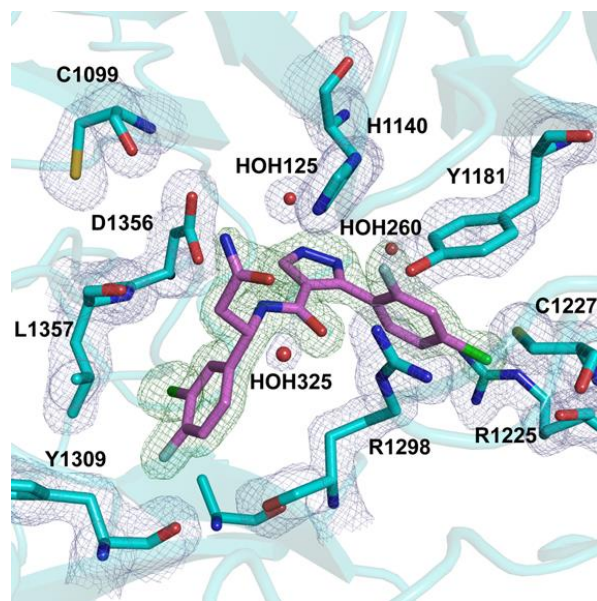
**Figure S2.** Orthogonal confirmation by ITC. The binding interaction between DCAF1 and original hit compound (Enamine, Z1391232269) was confirmed with an estimated  $K_D$  of 9  $\mu$ M. Experiment was performed in singlet.



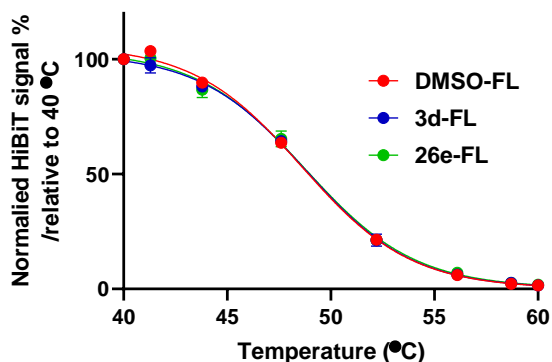
**Figure S3. Analysis of co-crystal structure of DCAF1 WDR domain in complex with two enantiomers.** Co-crystal structure showed the hit compound with R-configuration (in green) bound to DCAF1 with suboptimal geometry around the central amide function (neither trans nor cis configuration). Molecular modeling refinements showed the alternate enantiomer (S-configuration in orange) is a better fit of the co-crystal structure, while exhibiting optimal internal conformation.



**Figure S4. Zoomed-in view of compound 3d binding site in chain A of DCAF1-3d.** The protein residues in the vicinity of the compound are shown as sticks in light grey, the water molecule is depicted as a red sphere and the measured 2Fo-Fc electron density map is shown as grey mesh, contoured at 1.0 $\sigma$  level. The electron density omit map (Fo-Fc) shown as green mesh contoured at 3 $\sigma$  level corresponds to compound 3d (shown as yellow sticks).



**Figure S5. Zoomed-in view of the compound 26e binding site in chain A of DCAF1-26e.** The protein residues in the binding site are shown as cyan sticks, water molecules are rendered as red spheres and the measured 2Fo-Fc electron density map is shown as grey mesh, contoured at 1.0 $\sigma$  level. The electron density omit map (Fo-Fc) shown as green mesh contoured at 3 $\sigma$  level corresponds to the **26e** compound (shown as magenta sticks).



**Figure S6.** No target engagement observed for full length DCAF1. Neither **3d** nor **26e** were able to thermally stabilize full length DCAF1 at 40  $\mu$ M. Results shown as average  $\pm$  SD (n=3).

**Table S1.** Concentration-dependent stabilization of DCAF1 WD domain by compound **26e**

Compound <b>26e</b> ( $\mu$ M)	$\Delta T_m$ ( $^{\circ}$ C)
100	7.4 $\pm$ 0.5
50	6.9 $\pm$ 0.4
25	5.8 $\pm$ 0.3
12.5	3.3 $\pm$ 0.1
6.25	1.6 $\pm$ 0.1
3.125	0.8 $\pm$ 0.3

## 1. Report: Enantiomeric Excess of Compounds 3c (407) & 3d (406) (Lotus Separations)

### Chiral SFC Analyses for Enantiomeric Excess

<b>Title:</b>	Chiral SFC Analysis for Enantiomeric Excess Determination		
<b>Sample Name:</b>	Rac, 168b, 168c, 406 and 407	<b>Date:</b>	28-Sep-2021
<b>Requestor:</b>	Peter Brown	<b>Company:</b>	SGC, Univ of Toronto

#### Summary

Analyses for enantiomeric excess (ee) determination were requested for samples, 168b, 168c, 406 and 407 with the racemate provided. Chiral SFC separation conditions were developed and used, as described under Experimental Details below. The ee results are tabulated below.

Sample ID	Enantiomeric excess (ee)
168b	91.3%
168c	92.5%
406	96.8% (opposite enantiomer)
407	92.3%

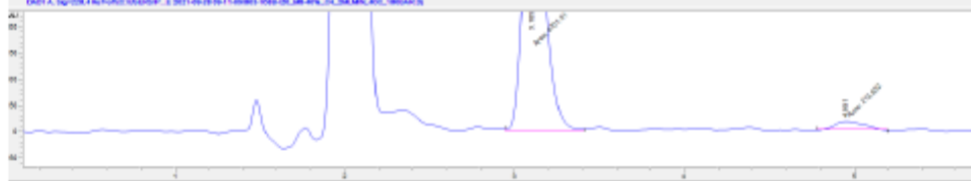
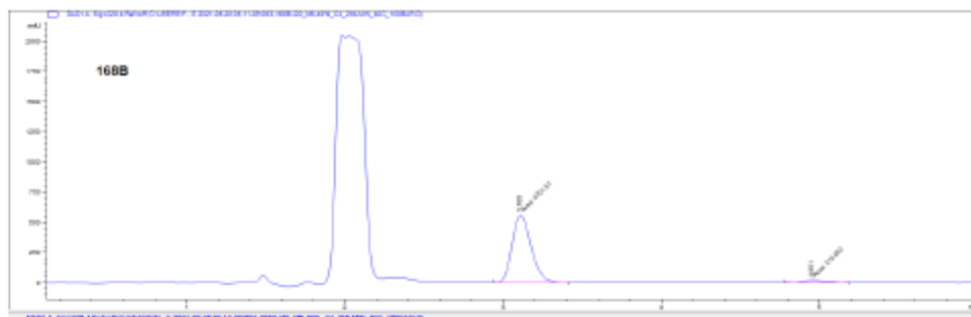
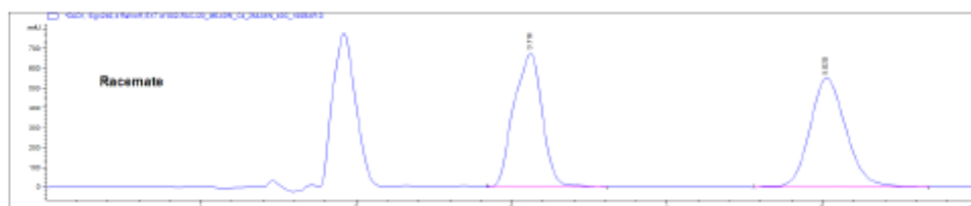
The chromatograms and integration results are shown in the following pages. The ID of the peaks were based on the retention match between the peaks in the racemate provided and those in the samples.

#### Experimental Details

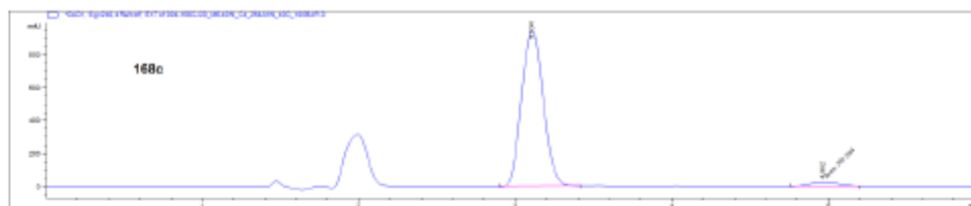
<b>SFC Analytical Conditions</b>	Instrument:	Agilent Aurora SFC
	Column:	Enantiocel A6-5 5µm, 250(L) x 4.6(ID) mm
	Temperature:	Ambient
	Flow rate:	2 mL/min
	Mobile Phase:	40% EtOH with 0.1% diethyl amine / 60% CO <sub>2</sub>
	Back-Pressure:	100 bar
	Injection volume:	15 µL
<b>Sample Prep.:</b>	1:1 dilution with MeOH of the 20mM DMSO sample solutions provided	

OICR0036766A02	BJW-0010-0406-05	20 mM	406	as much as you can supply	S
OICR0036767A02	BJW-0010-0407-05	20 mM	407	as much as you can supply	R
	mixture of 2 above solns	20 mM	racemic	150 microL of each mixed	RS
	UB023168b	20 mM	168b	as much as you can supply	R
	UB023168c	20 mM	168c	as much as you can supply	R

Chromatograms and Results:



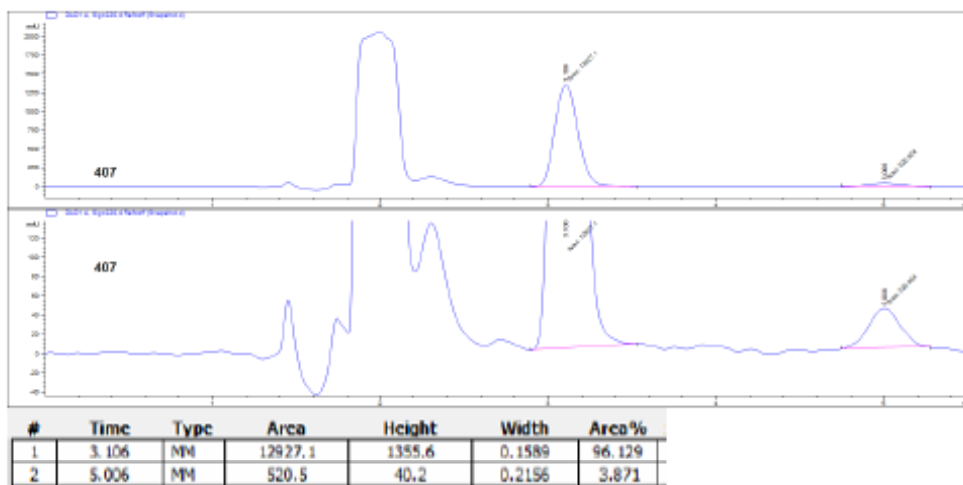
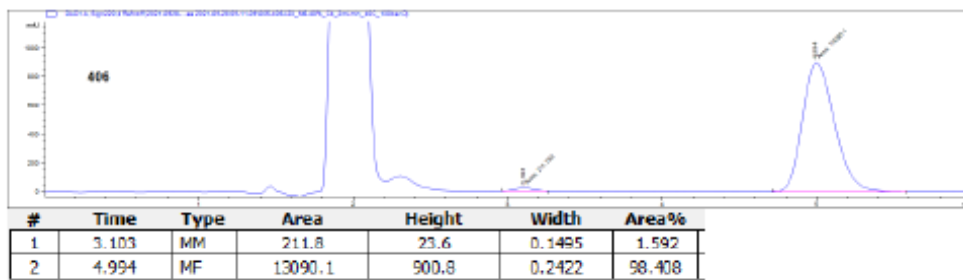
#	Time	Type	Area	Height	Width	Area%
1	3.105	MF	4701.5	557.3	0.1406	95.653
2	4.951	MM	213.7	17.1	0.2084	4.347



#	Time	Type	Area	Height	Width	Area%
1	3.104	VB	9121.1	947.2	0.1543	96.233
2	4.962	MM	357.1	26.4	0.225	3.767

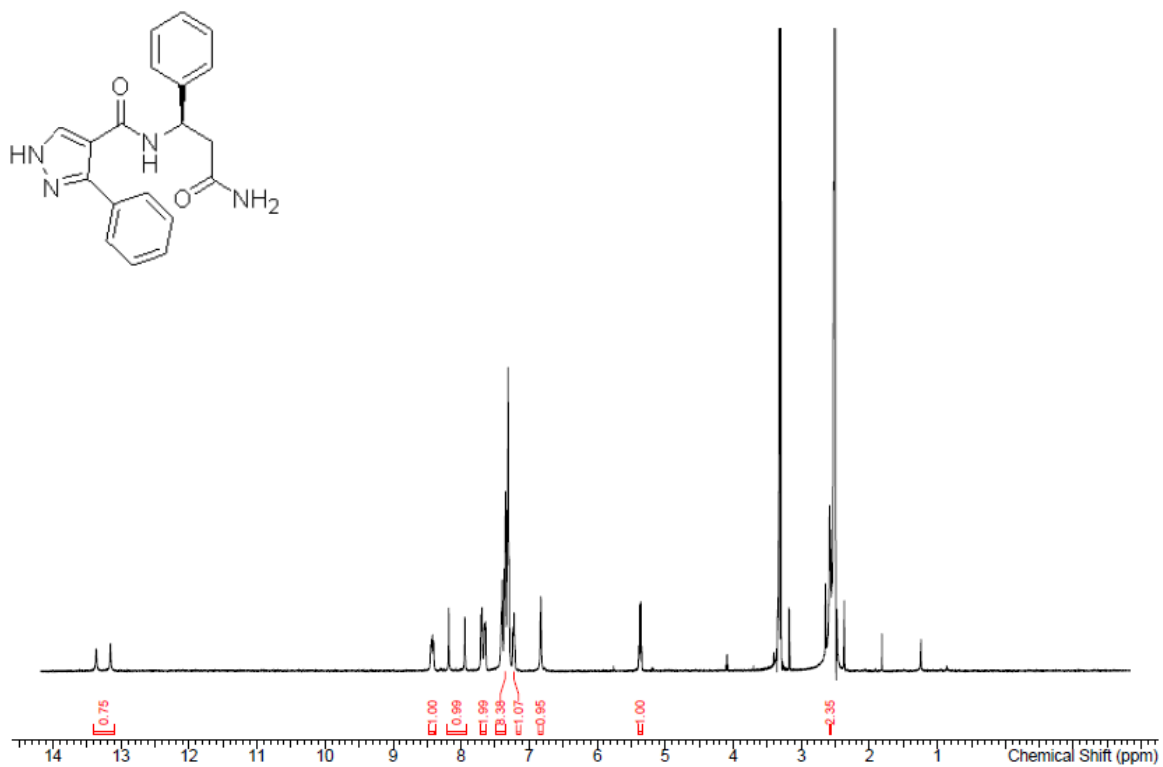


### Chiral SFC Analyses for Enantiomeric Excess

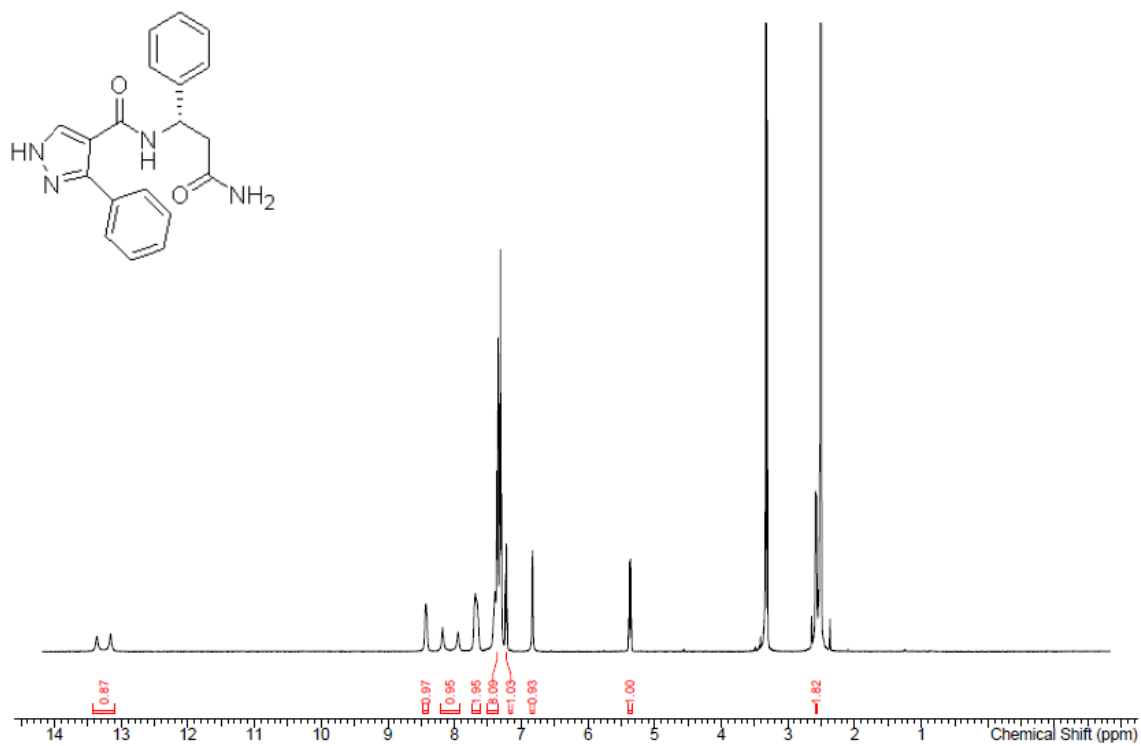


## 2. $^1\text{H}$ NMR Spectra for tested compounds

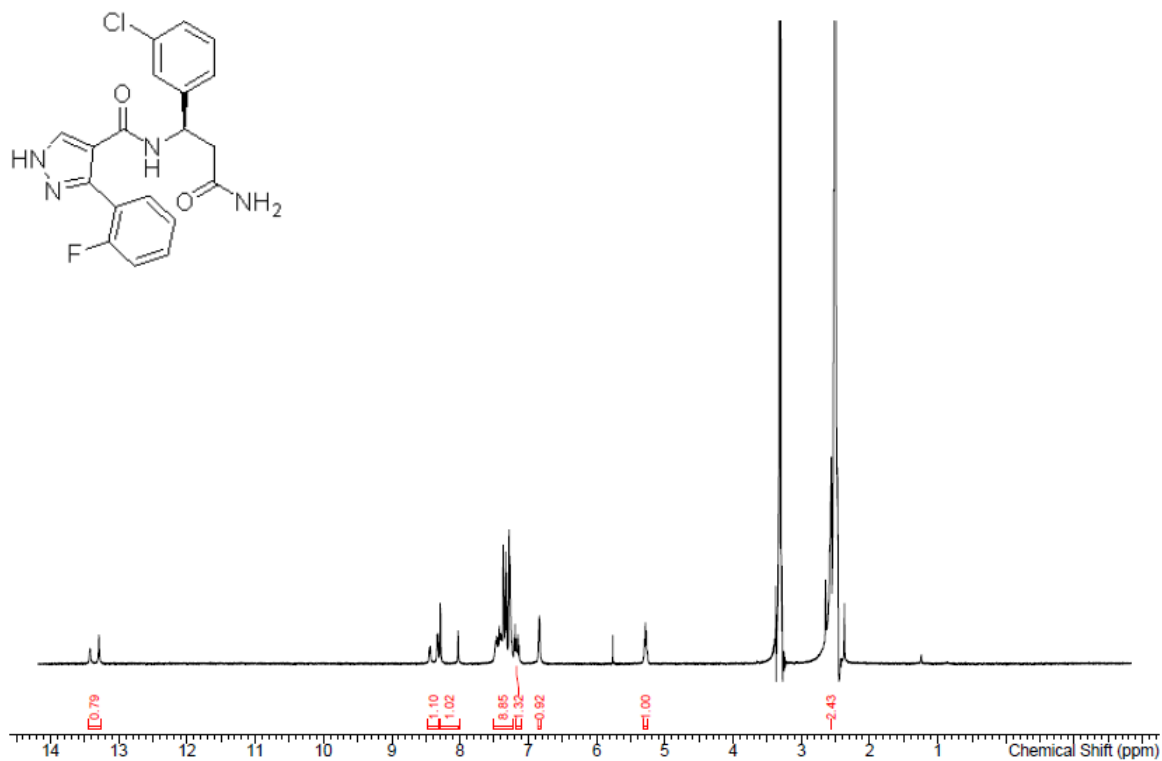
$^1\text{H}$  NMR Spectrum for compound **3a** (DMSO- $d_6$ , 500 MHz)



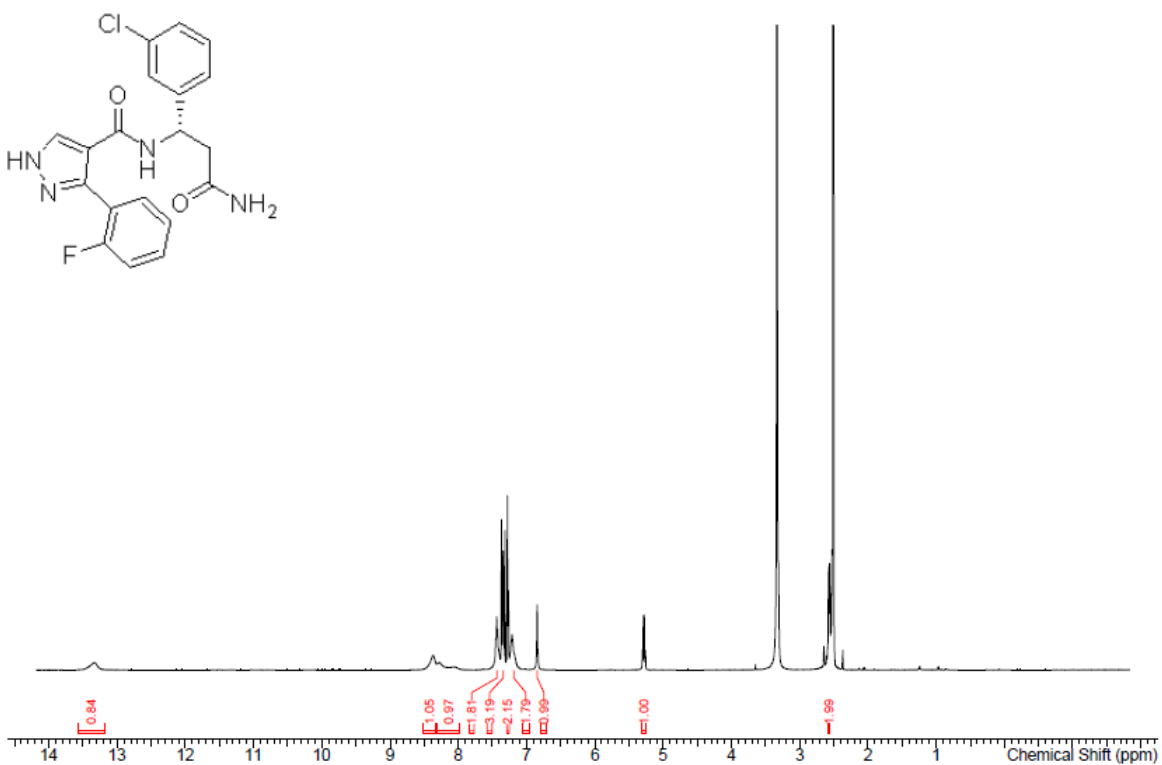
$^1\text{H}$  NMR Spectra for compound **3b** (DMSO- $d_6$ , 500 MHz)



<sup>1</sup>H NMR Spectra for compound **3c** (DMSO-*d*<sub>6</sub>, 500 MHz)

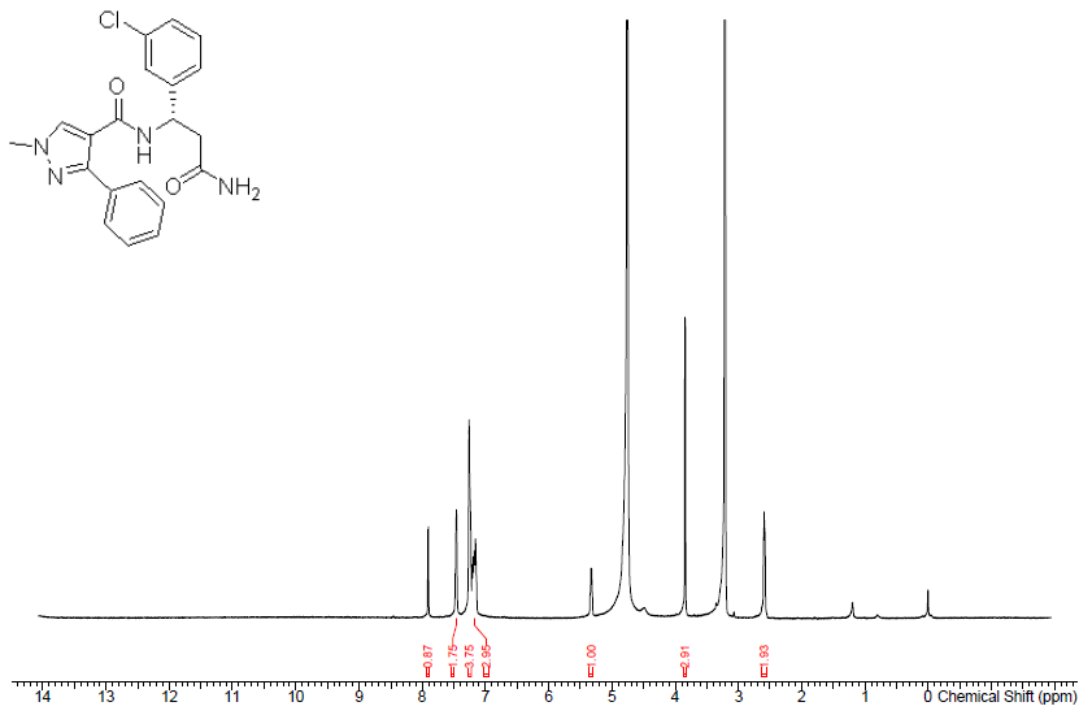


<sup>1</sup>H NMR Spectra for compound **3d** (DMSO-*d*<sub>6</sub>, 500 MHz)



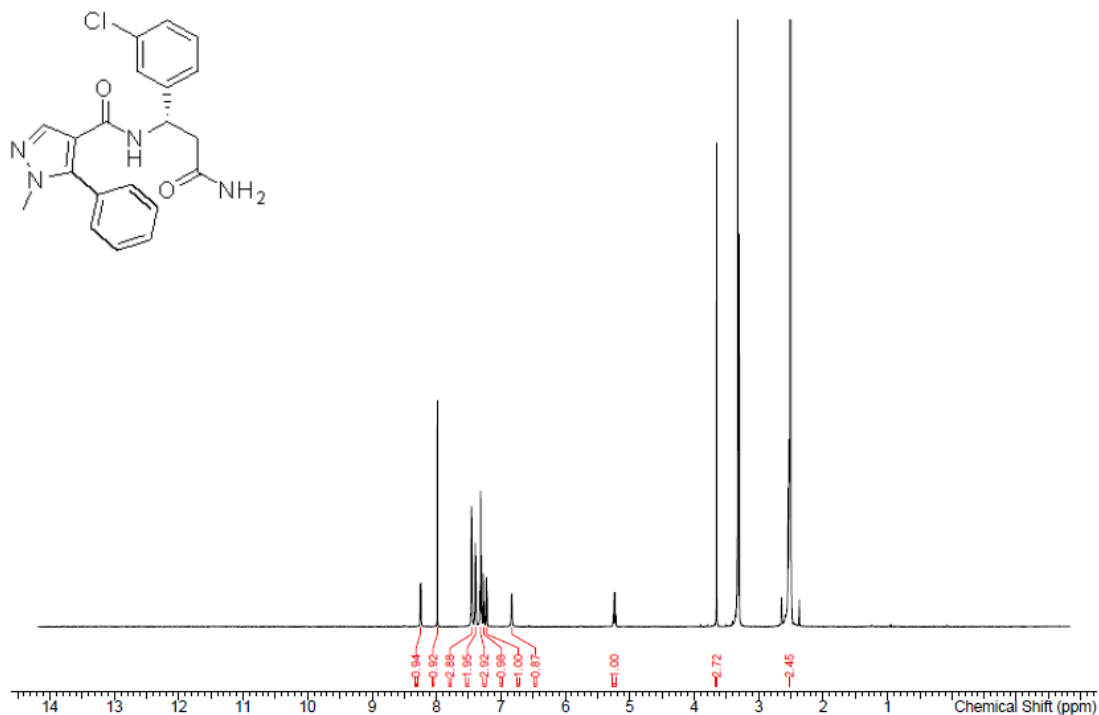
### <sup>1</sup>H NMR Spectra for compound **5a** (MeOH-*d*<sub>4</sub>, 500 MHz)

<sup>1</sup>H NMR (METHANOL-*d*<sub>4</sub>, 500 MHz) δ 7.91 (d, 1H, *J*=4.5 Hz), 7.48-7.44 (m, 2H), 7.28-7.22 (m, 4H), 7.22-7.13 (m, 3H), 5.36-5.30 (m, 1H), 3.84 (d, 3H, *J*=4.6 Hz), 2.63-2.56 (m, 2H)



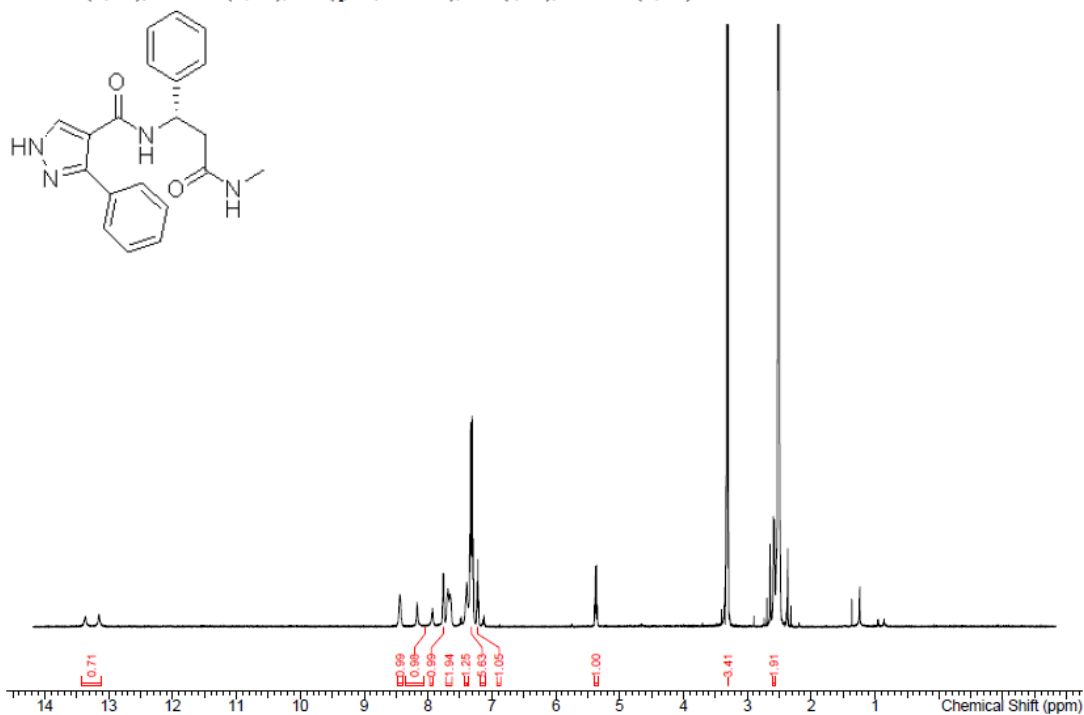
### <sup>1</sup>H NMR Spectra for compound **5b** (DMSO-*d*<sub>6</sub>, 500 MHz)

<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz) δ 8.25 (d, 1H, *J*=8.1 Hz), 7.99 (s, 1H), 7.48-7.44 (m, 3H), 7.41-7.38 (m, 2H), 7.34-7.29 (m, 3H), 7.28-7.25 (m, 1H), 7.23-7.21 (m, 1H), 6.83 (br s, 1H), 5.24 (q, 1H, *J*=7.3 Hz), 3.65 (s, 3H), 2.54-2.52 (m, 2H)



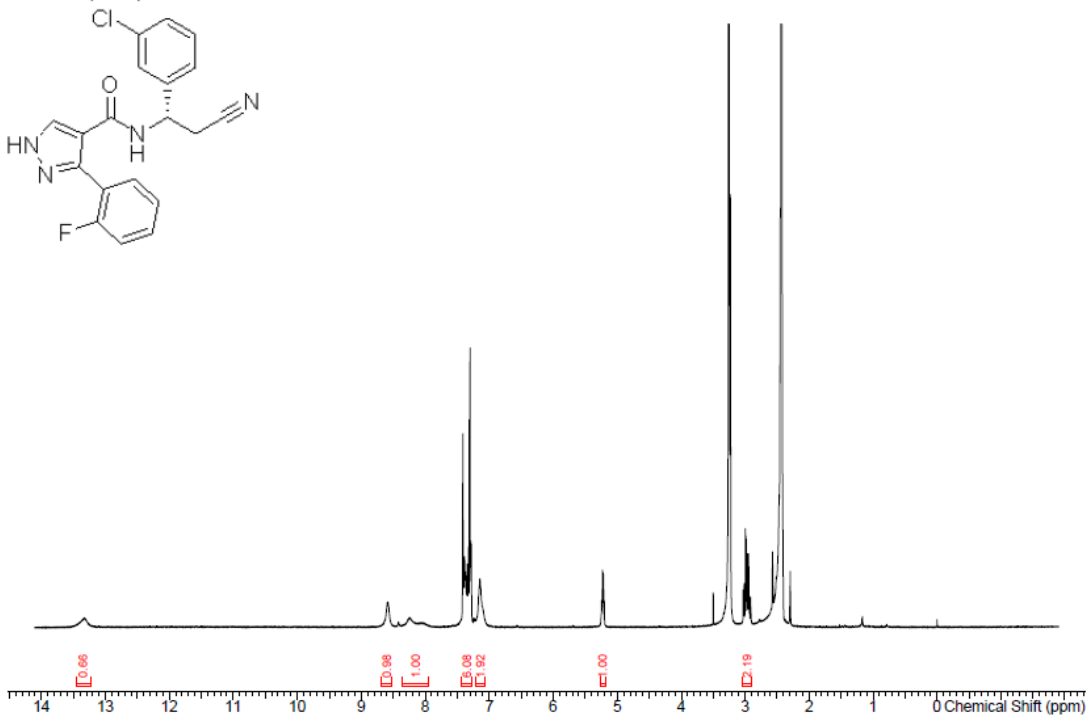
### <sup>1</sup>H NMR Spectra for compound **5c** (DMSO-*d*<sub>6</sub>, 500 MHz)

<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz) δ 13.41-13.11 (m, 1H), 8.44 (br s, 1H), 8.19-7.90 (m, 1H), 7.78-7.74 (m, 1H), 7.72-7.62 (m, 2H), 7.40 (br s, 1H), 7.37-7.28 (m, 6H), 7.25-7.20 (m, 1H), 5.37 (q, 1H, *J*=7.5 Hz), 3.30 (s, 3H), 2.60-2.57 (m, 2H)



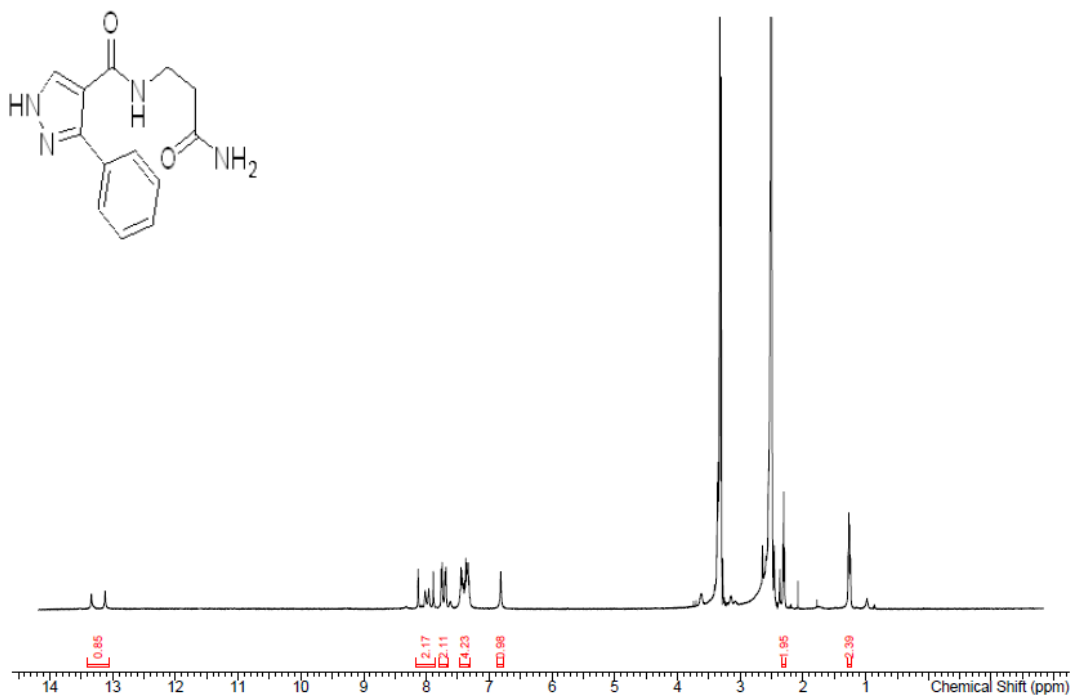
### <sup>1</sup>H NMR Spectra for compound **5d** (DMSO-*d*<sub>6</sub>, 500 MHz)

<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz) δ 13.34 (b s, 1H), 8.59 (b s, 1H), 8.36-7.95 (b m, 1H), 7.43-7.27 (m, 6H), 7.14 (b s, 2H), 5.26-5.19 (m, 1H), 3.04-2.90 (m, 2H)



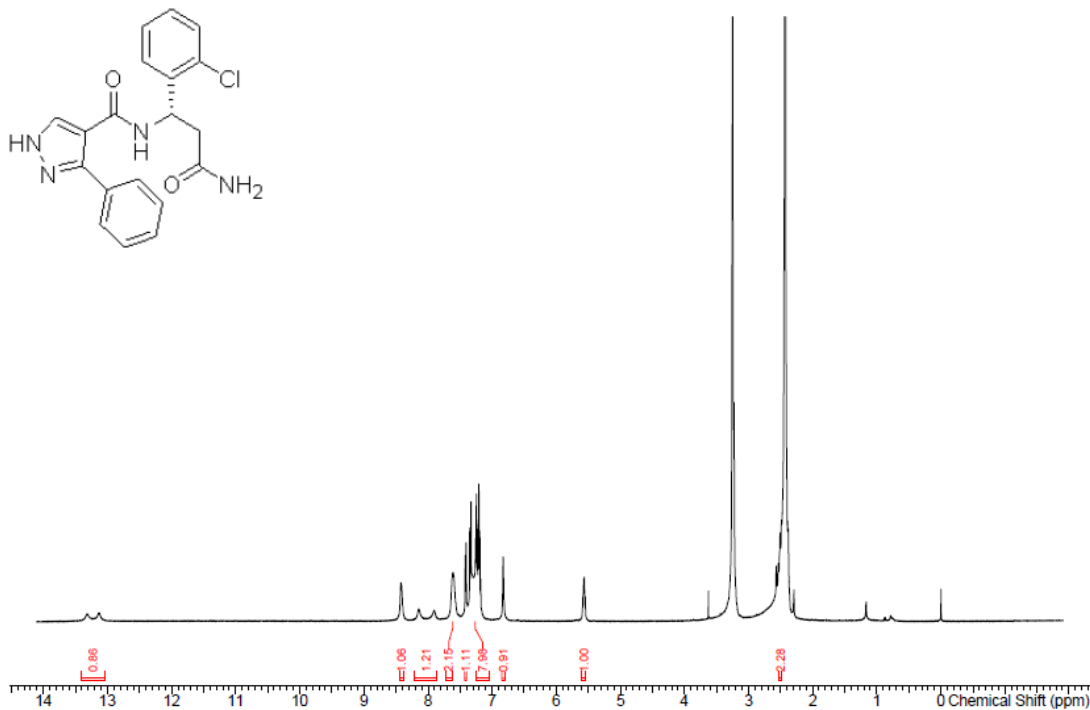
### <sup>1</sup>H NMR Spectra for compound **14a** (DMSO-*d*<sub>6</sub>, 500 MHz)

<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz) δ 13.37-13.07 (m, 1H), 8.16-7.86 (m, 2H), 7.80-7.66 (m, 2H), 7.47-7.31 (m, 4H), 6.82 (br s, 1H), 2.31 (t, 2H, *J*=7.2 Hz), 1.29-1.24 (m, 2H)



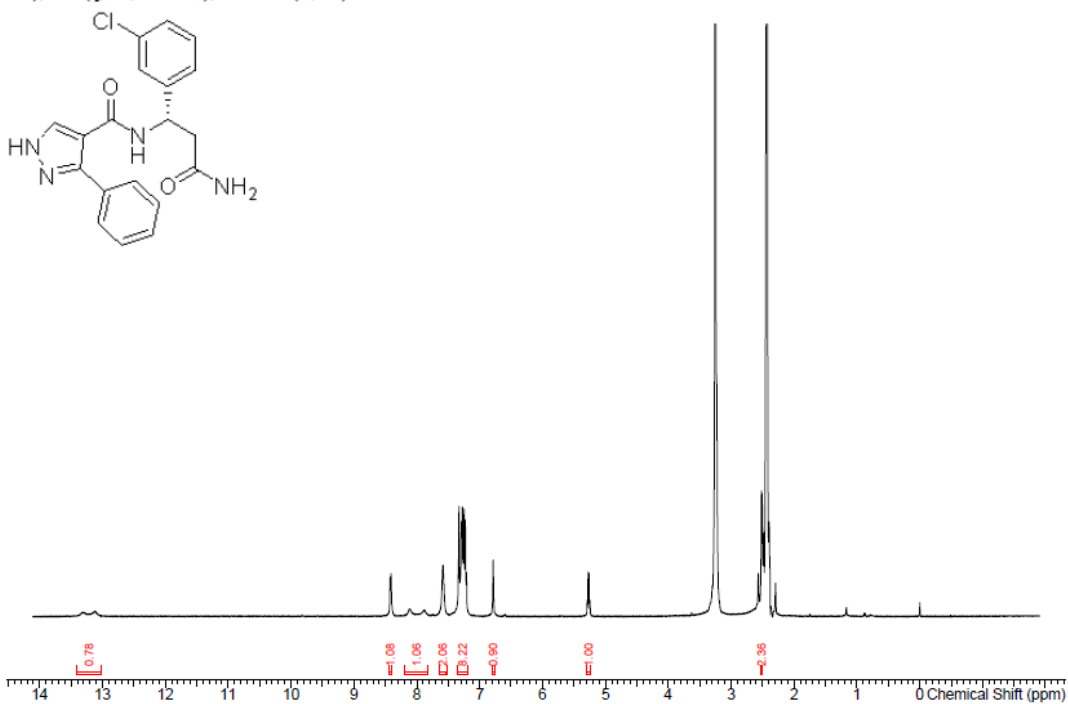
### <sup>1</sup>H NMR Spectra for compound **14b** (DMSO-*d*<sub>6</sub>, 500 MHz)

<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz) δ 13.41-13.05 (m, 1H), 8.42 (br s, 1H), 8.21-7.86 (m, 1H), 7.61 (br s, 2H), 7.41 (br d, 1H, *J*=6.8 Hz), 7.36-7.17 (m, 8H), 6.83 (br s, 1H), 5.60-5.53 (m, 1H), 2.52-2.48 (m, 2H)



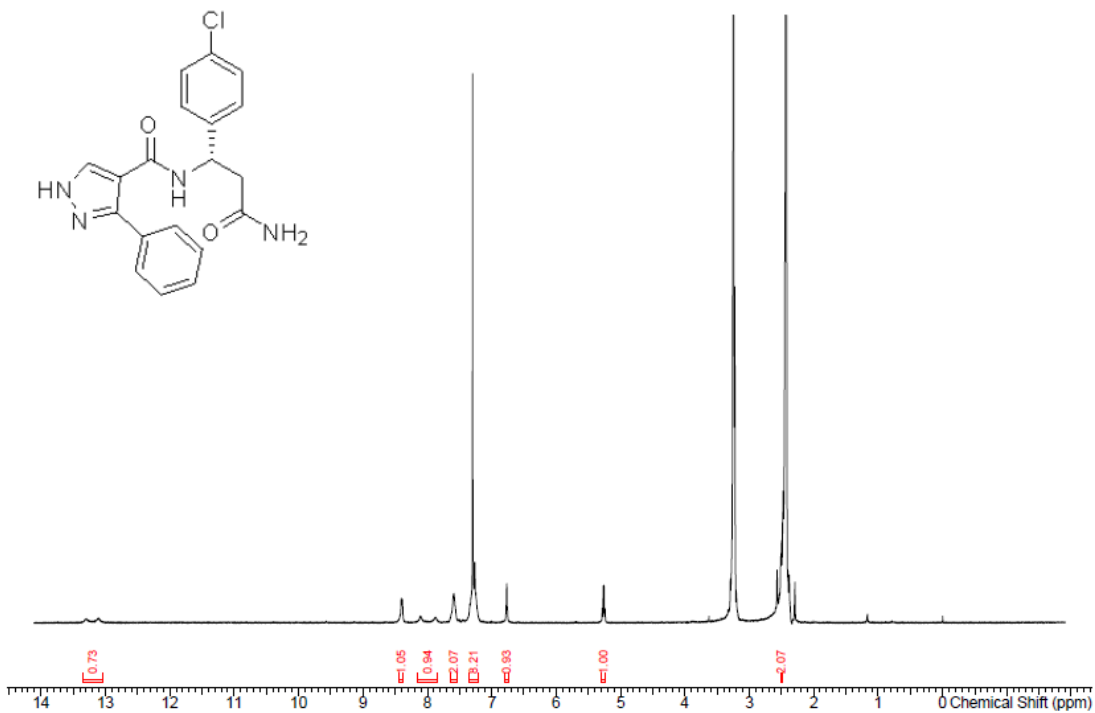
### <sup>1</sup>H NMR Spectra for compound **14c** (DMSO-*d*<sub>6</sub>, 500 MHz)

<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz) δ 13.40-13.04 (m, 1H), 8.42 (br d, 1H, *J*=8.1 Hz), 8.18-7.82 (m, 1H), 7.58 (br s, 2H), 7.35-7.19 (m, 8H), 6.79 (br s, 1H), 5.27 (q, 1H, *J*=7.5 Hz), 2.53-2.50 (m, 2H)



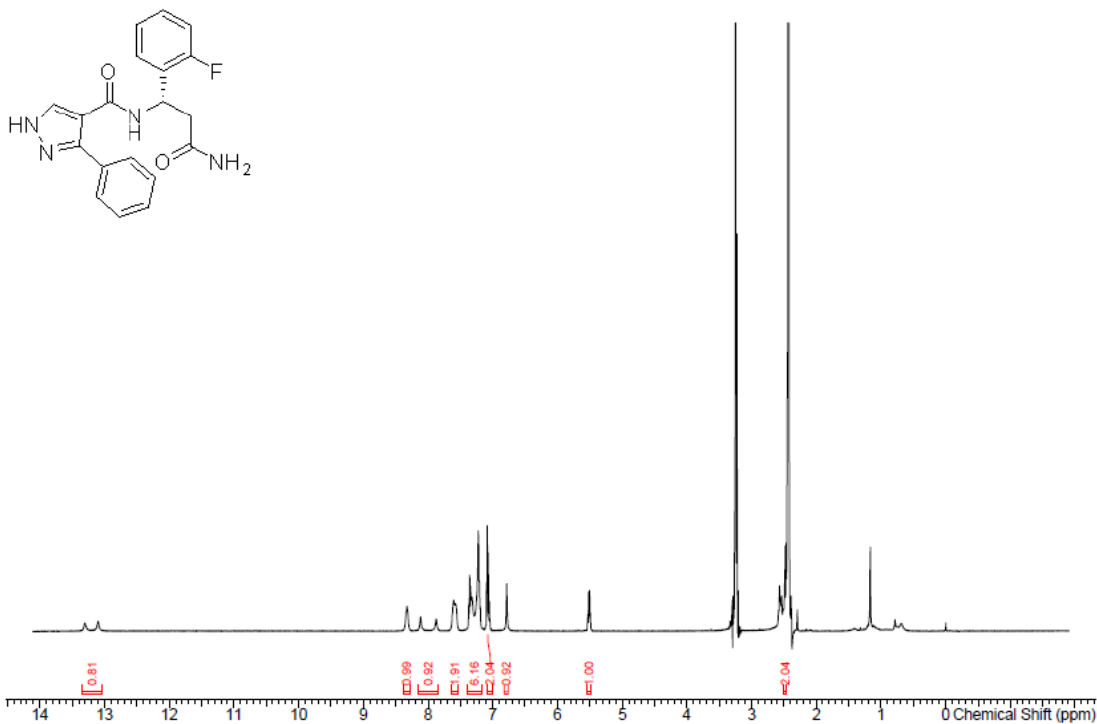
### <sup>1</sup>H NMR Spectra for compound **14d** (DMSO-*d*<sub>6</sub>, 500 MHz)

<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz) δ 13.35-13.05 (m, 1H), 8.40 (br d, 1H, *J*=7.9 Hz), 8.16-7.83 (m, 1H), 7.59 (br s, 2H), 7.36-7.22 (m, 8H), 6.77 (br s, 1H), 5.26 (q, 1H, *J*=7.5 Hz), 2.52-2.49 (m, 2H)



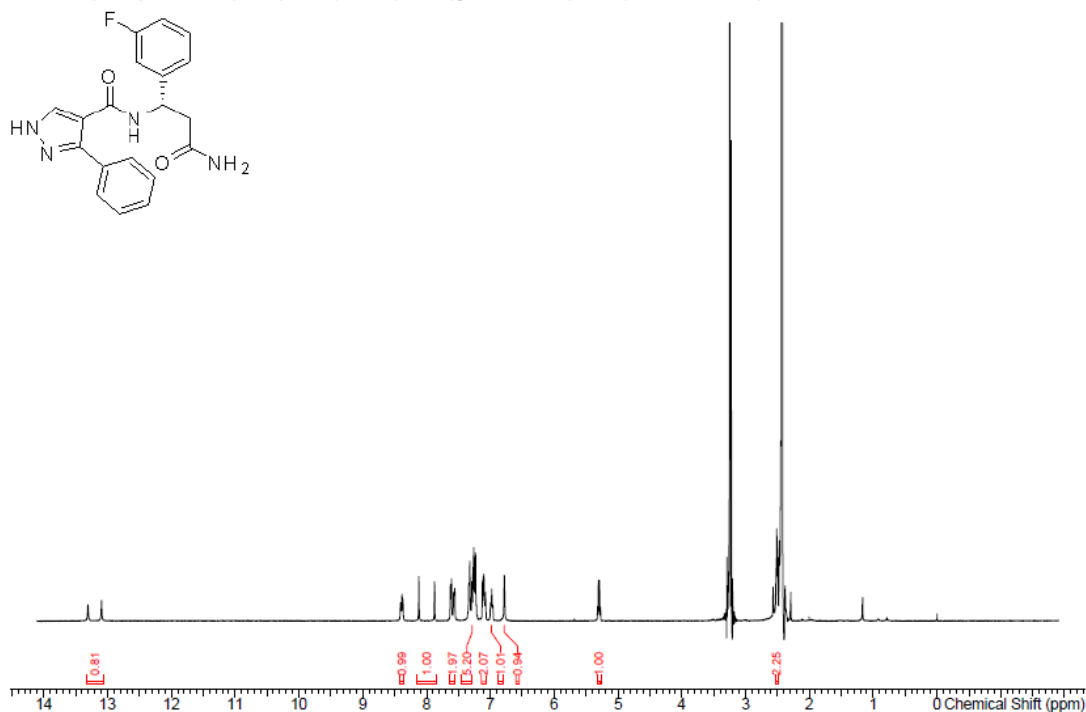
### <sup>1</sup>H NMR Spectra for compound **14e** (DMSO-*d*<sub>6</sub>, 500 MHz)

<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz) δ 13.36-13.04 (m, 1H), 8.33 (br s, 1H), 8.15-7.84 (m, 1H), 7.65-7.54 (m, 2H), 7.39-7.17 (m, 6H), 7.12-7.03 (m, 2H), 6.78 (br s, 1H), 5.55-5.48 (m, 1H), 2.50-2.46 (m, 2H)



### <sup>1</sup>H NMR Spectra for compound **14f** (DMSO-*d*<sub>6</sub>, 500 MHz)

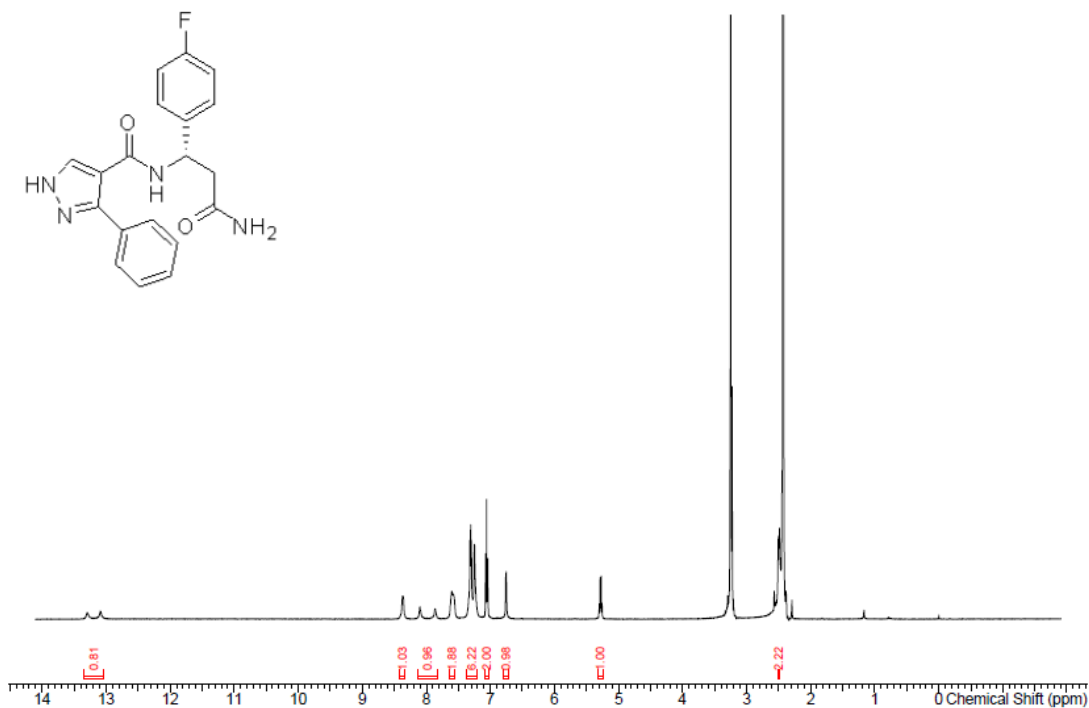
<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz) δ 13.33-13.07 (m, 1H), 8.39 (br dd, 1H, *J*=8.7, 11.4 Hz), 8.15-7.84 (m, 1H), 7.64-7.54 (m, 2H), 7.36-7.21 (m, 5H), 7.14-7.06 (m, 2H), 7.02-6.95 (m, 1H), 6.78 (br s, 1H), 5.30 (q, 1H, *J*=7.6 Hz), 2.51 (br t, 2H, *J*=6.6 Hz)





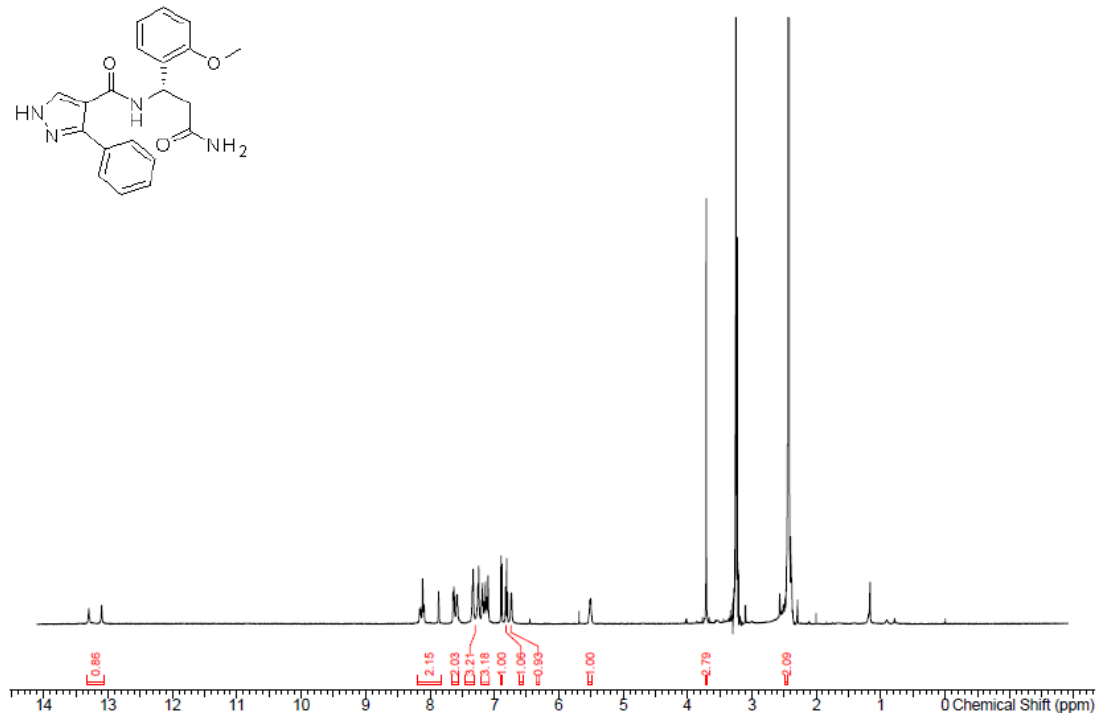
### <sup>1</sup>H NMR Spectra for compound **14g** (DMSO-*d*<sub>6</sub>, 500 MHz)

<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz) δ 13.36-13.04 (m, 1H), 8.37 (br s, 1H), 8.13-7.83 (m, 1H), 7.65-7.55 (m, 2H), 7.37-7.21 (m, 6H), 7.06 (t, 2H, *J*=8.9 Hz), 6.76 (br s, 1H), 5.28 (q, 1H, *J*=7.6 Hz), 2.51-2.48 (m, 2H)



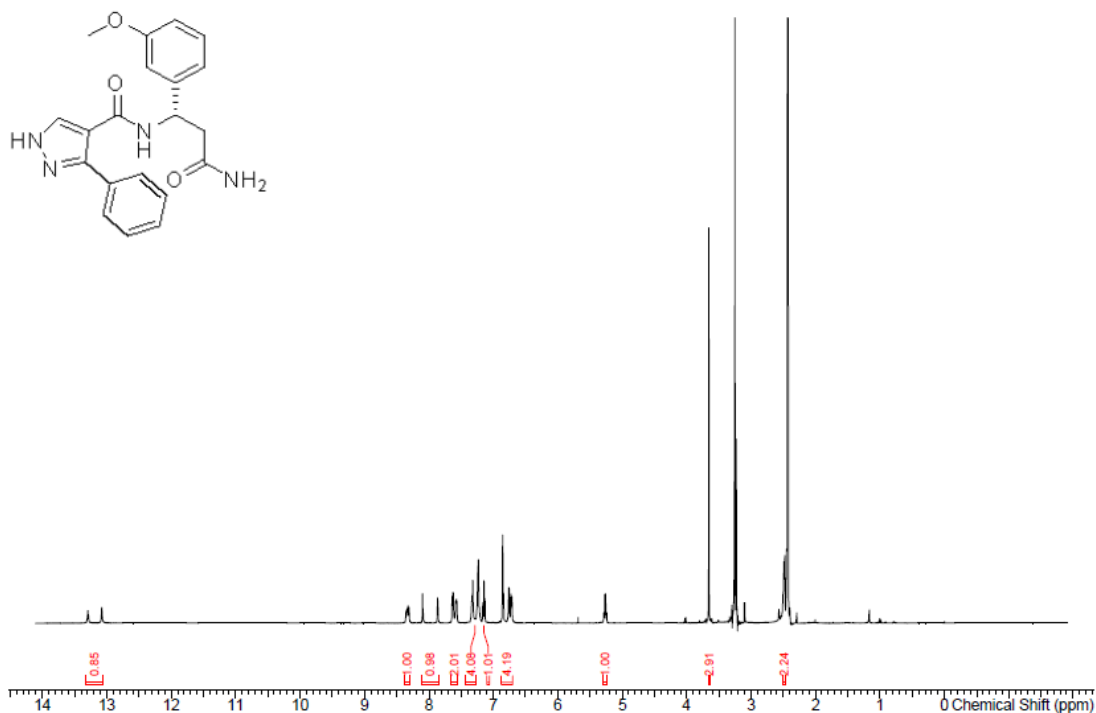
### <sup>1</sup>H NMR Spectra for compound **14h** (DMSO-*d*<sub>6</sub>, 500 MHz)

<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz) δ 13.33-13.07 (m, 1H), 8.18-7.84 (m, 2H), 7.65-7.56 (m, 2H), 7.37-7.22 (m, 3H), 7.21-7.08 (m, 3H), 6.89 (d, 1H, *J*=8.1 Hz), 6.81 (t, 1H, *J*=7.3 Hz), 6.74 (br s, 1H), 5.54-5.48 (m, 1H), 3.71 (s, 3H), 2.48-2.45 (m, 2H)



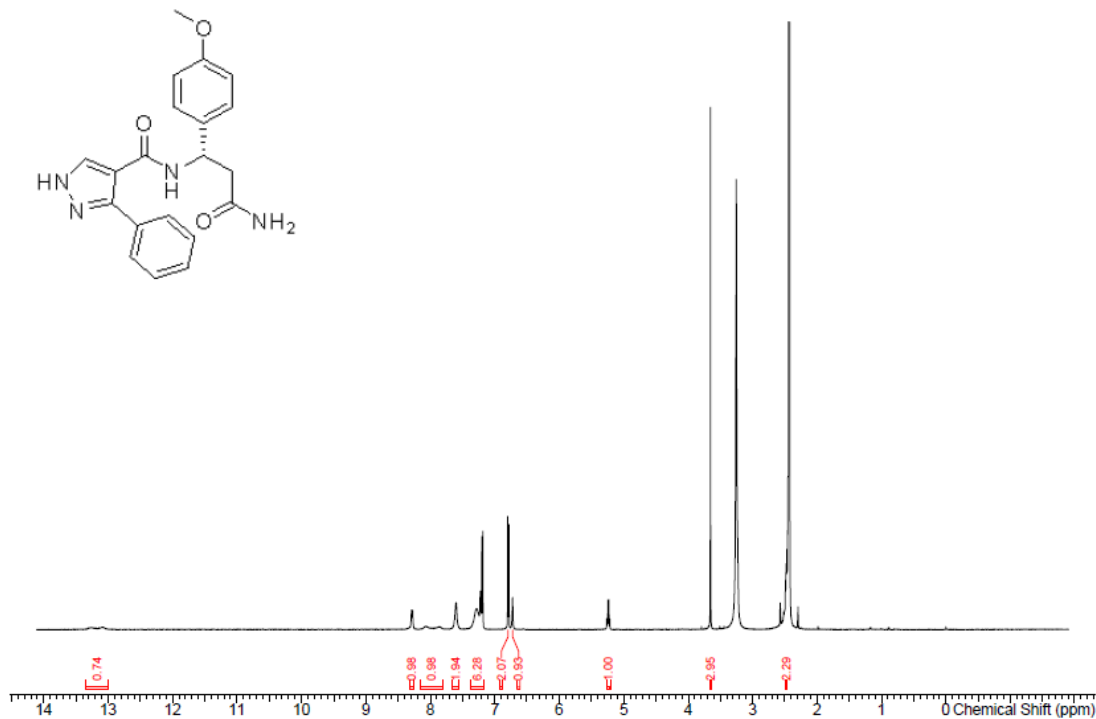
### <sup>1</sup>H NMR Spectra for compound **14i** (DMSO-*d*<sub>6</sub>, 500 MHz)

<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz) δ 13.33-13.05 (m, 1H), 8.33 (br dd, 1H, *J*=8.4, 14.6 Hz), 8.11-7.84 (m, 1H), 7.66-7.56 (m, 2H), 7.36-7.21 (m, 4H), 7.15 (t, 1H, *J*=7.8 Hz), 6.88-6.70 (m, 4H), 5.27 (q, 1H, *J*=7.5 Hz), 3.66 (s, 3H), 2.50-2.47 (m, 2H, *J*=6.5 Hz)



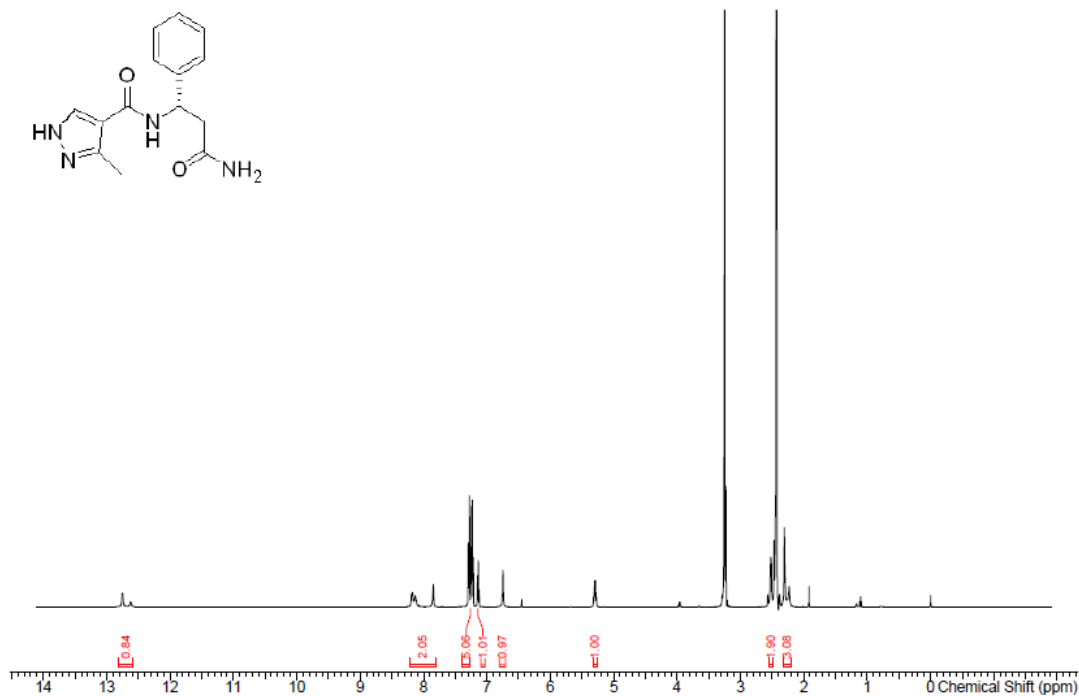
### <sup>1</sup>H NMR Spectra for compound **14j** (DMSO-*d*<sub>6</sub>, 500 MHz)

<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz) δ 13.36-13.00 (m, 1H), 8.28 (br d, 1H, *J*=8.2 Hz), 8.15-7.81 (m, 1H), 7.60 (br s, 2H), 7.37-7.17 (m, 6H), 6.82-6.77 (m, 2H), 6.72 (br s, 1H), 5.24 (q, 1H, *J*=7.5 Hz), 3.65 (s, 3H), 2.49-2.46 (m, 2H)



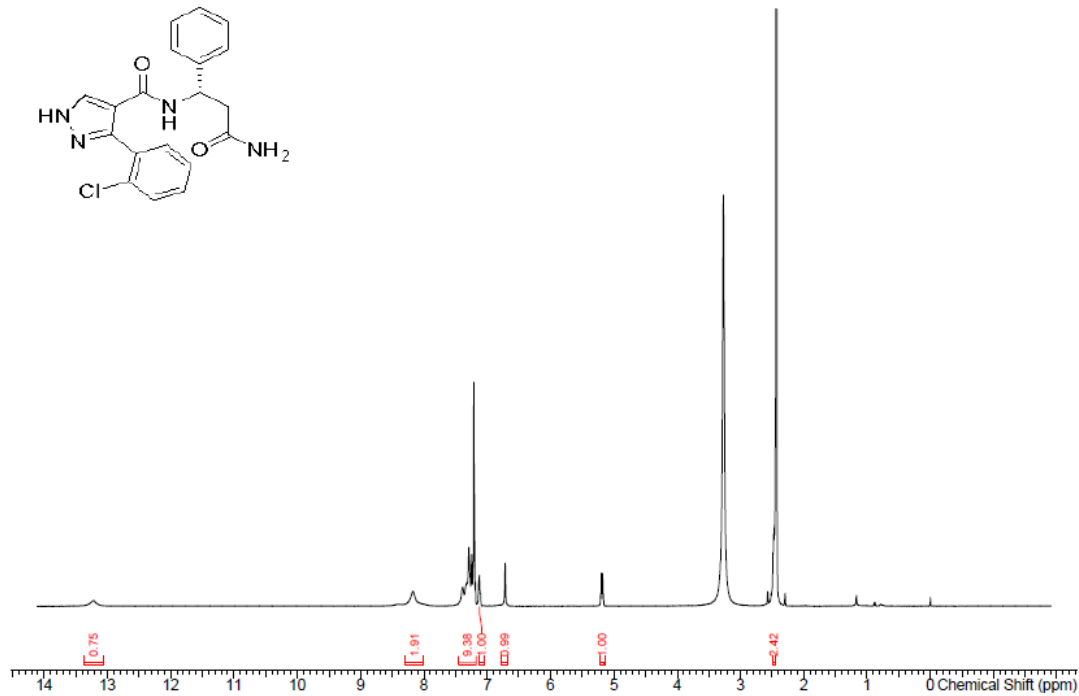
### $^1\text{H}$ NMR Spectra for compound **15a** (DMSO- $d_6$ , 500 MHz)

$^1\text{H}$  NMR (DMSO- $d_6$ , 500 MHz)  $\delta$  12.81-12.59 (m, 1H), 8.22-7.81 (m, 2H), 7.32-7.20 (m, 5H), 7.17-7.11 (m, 1H), 6.75 (br s, 1H), 5.29 (q, 1H,  $J=7.5$  Hz), 2.52 (br d, 2H,  $J=6.7$  Hz), 2.32-2.21 (m, 3H)



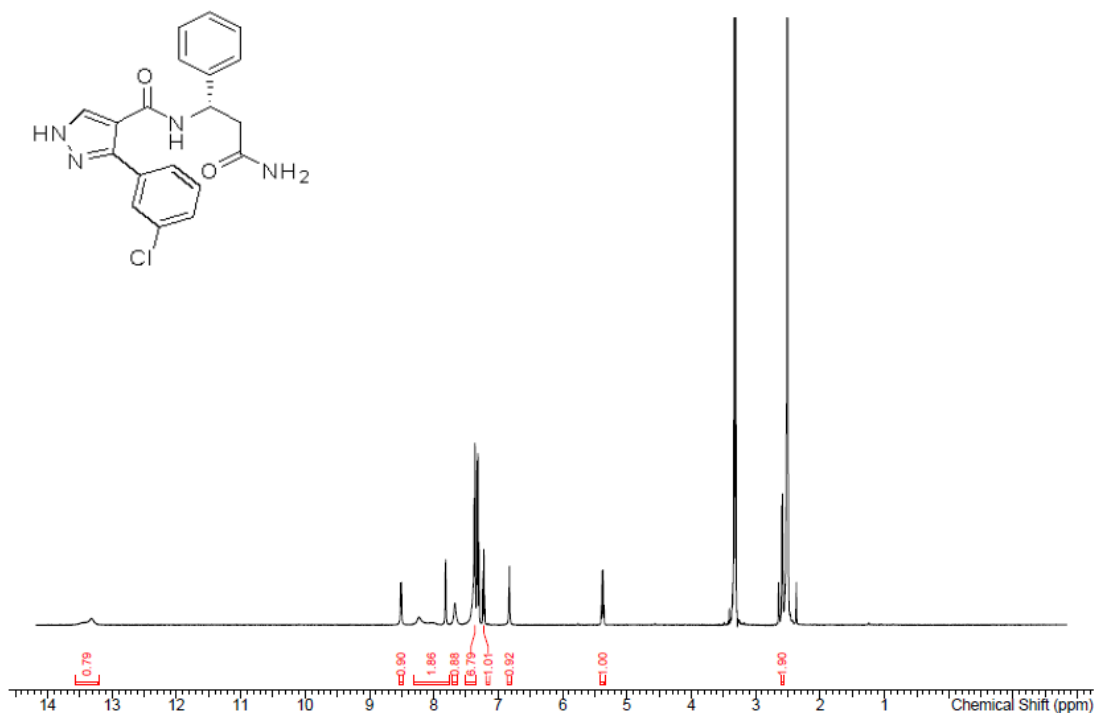
### $^1\text{H}$ NMR Spectra for compound **15b** (DMSO- $d_6$ , 500 MHz)

$^1\text{H}$  NMR (DMSO- $d_6$ , 500 MHz)  $\delta$  13.22 (br s, 1H), 8.16 (br s, 2H), 7.45-7.17 (m, 9H), 7.13 (br d, 1H,  $J=5.7$  Hz), 6.72 (br s, 1H), 5.19 (q, 1H,  $J=7.4$  Hz), 2.47 (br d, 2H,  $J=6.4$  Hz)



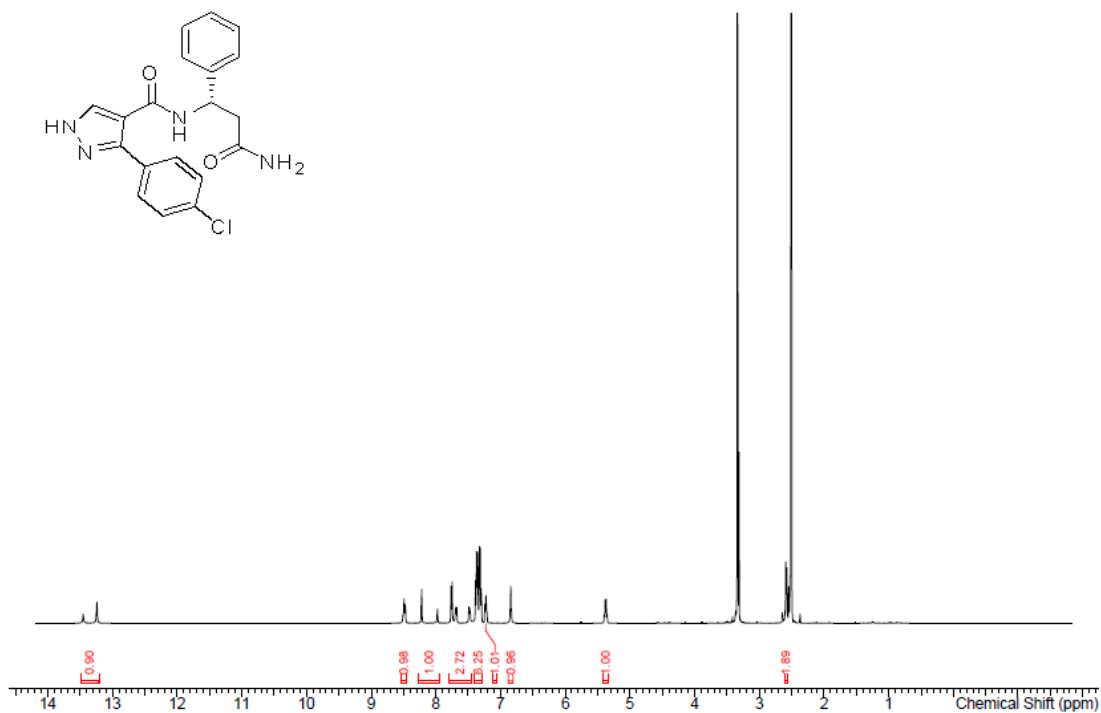
### <sup>1</sup>H NMR Spectra for compound **15c** (DMSO-*d*<sub>6</sub>, 500 MHz)

<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz) δ 13.57-13.21 (m, 1H), 8.51 (br d, 1H, *J*=8.2 Hz), 8.31-7.77 (m, 2H), 7.67 (br s, 1H), 7.44-7.28 (m, 7H), 7.25-7.20 (m, 1H), 6.83 (br s, 1H), 5.38 (q, 1H, *J*=7.5 Hz), 2.59 (br d, 2H, *J*=7.3 Hz)



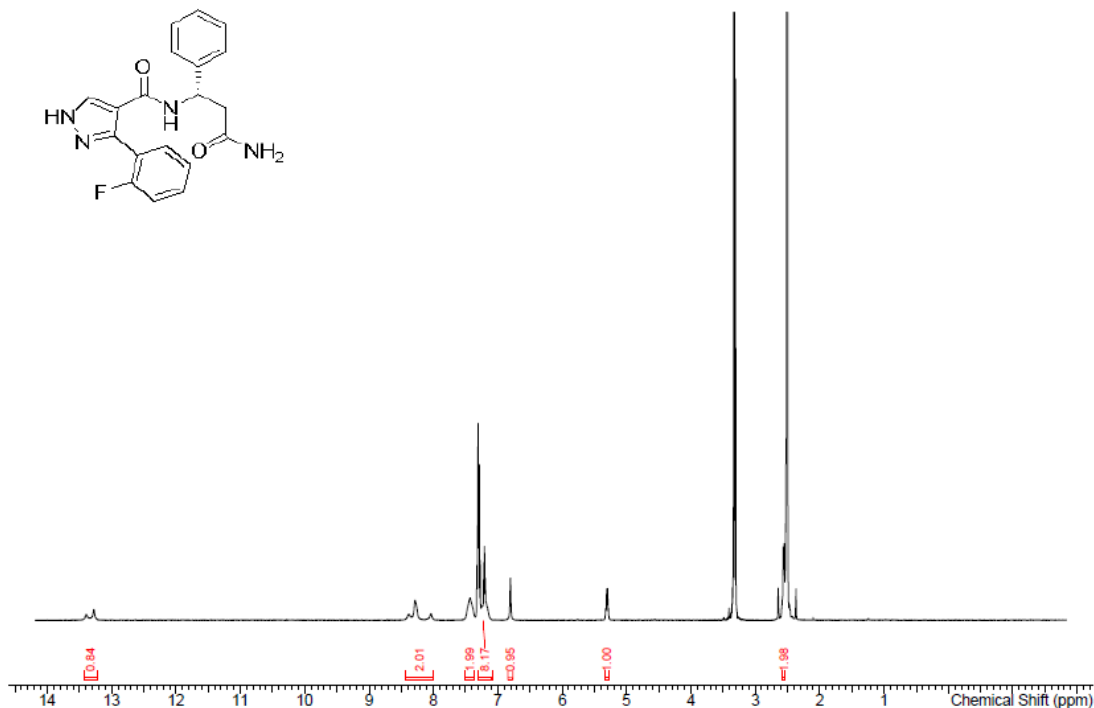
### <sup>1</sup>H NMR Spectra for compound **15d** (DMSO-*d*<sub>6</sub>, 500 MHz)

<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz) δ 13.50-13.21 (m, 1H), 8.53-8.46 (m, 1H), 8.28-7.95 (m, 1H), 7.80-7.45 (m, 3H), 7.41-7.29 (m, 6H), 7.26-7.20 (m, 1H), 6.84 (br s, 1H), 5.38 (q, 1H, *J*=7.5 Hz), 2.58 (br d, 2H, *J*=7.2 Hz)



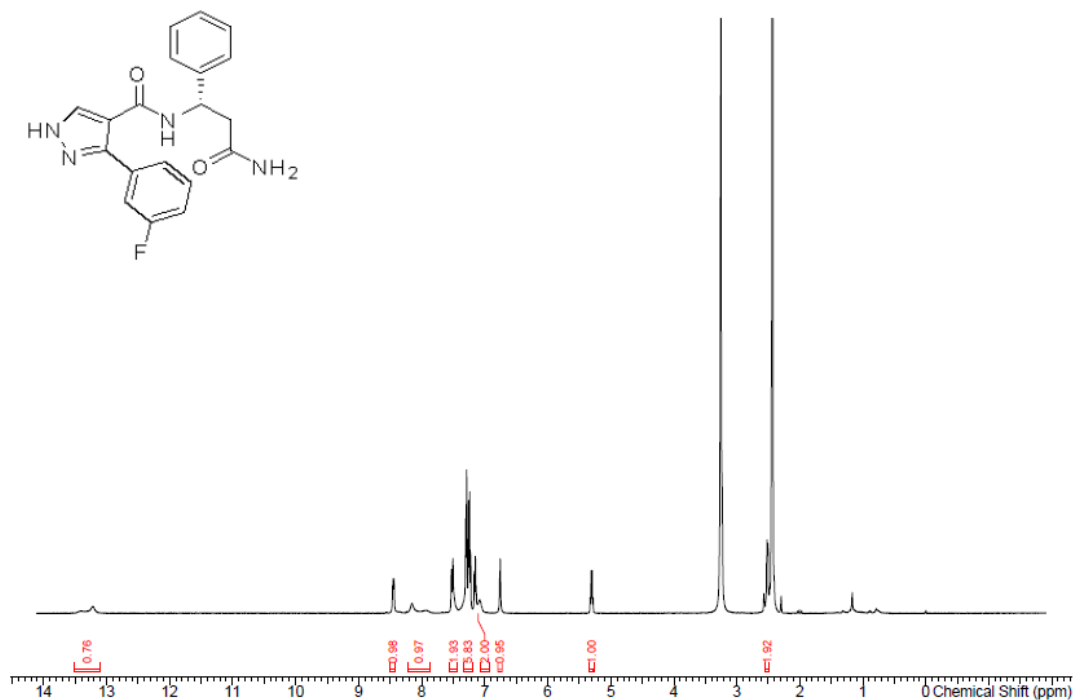
### <sup>1</sup>H NMR Spectra for compound **15e** (DMSO-*d*<sub>6</sub>, 500 MHz)

<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz) δ 13.43-13.22 (m, 1H), 8.44-8.00 (m, 2H), 7.43 (br s, 2H), 7.34-7.12 (m, 8H), 6.80 (br s, 1H), 5.30 (q, 1H, *J*=7.3 Hz), 2.56 (br d, 2H, *J*=6.8 Hz)



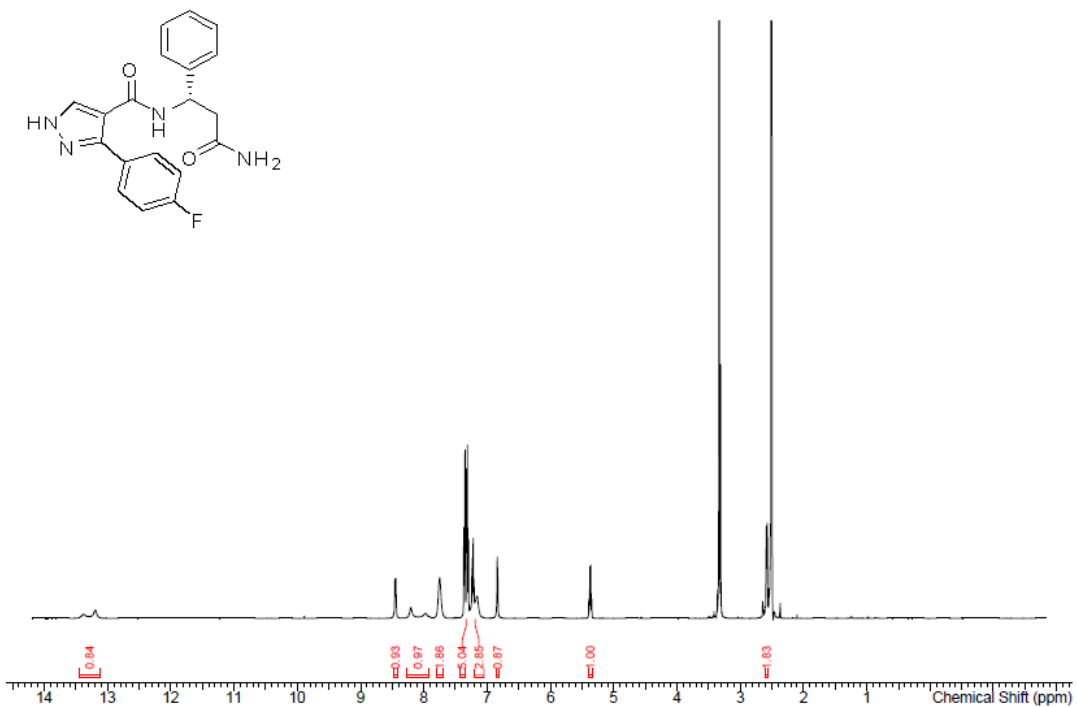
### <sup>1</sup>H NMR Spectra for compound **15f** (DMSO-*d*<sub>6</sub>, 500 MHz)

<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz) δ 13.52-13.10 (m, 1H), 8.45 (br d, 1H, *J*=7.7 Hz), 8.22-7.86 (m, 1H), 7.55-7.43 (m, 2H), 7.32-7.20 (m, 6H), 7.18-7.03 (m, 2H), 6.75 (br s, 1H), 5.30 (q, 1H, *J*=7.5 Hz), 2.51 (br dd, 2H, *J*=3.5, 6.8 Hz)



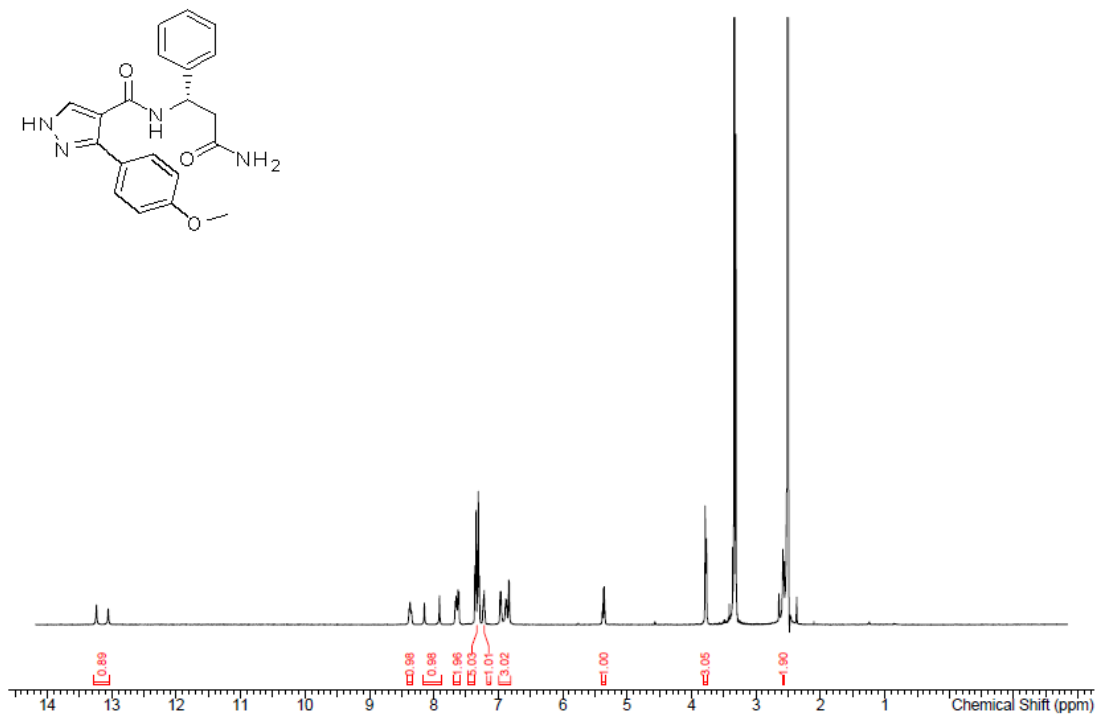
<sup>1</sup>H NMR Spectra for compound **15g** (DMSO-*d*<sub>6</sub>, 500 MHz)

<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz) δ 13.44-13.12 (m, 1H), 8.45 (br d, 1H, *J*=8.1 Hz), 8.26-7.92 (m, 1H), 7.75 (br s, 2H), 7.38-7.29 (m, 5H), 7.26-7.11 (m, 3H), 6.84 (br s, 1H), 5.37 (q, 1H, *J*=7.5 Hz), 2.60-2.56 (m, 2H)



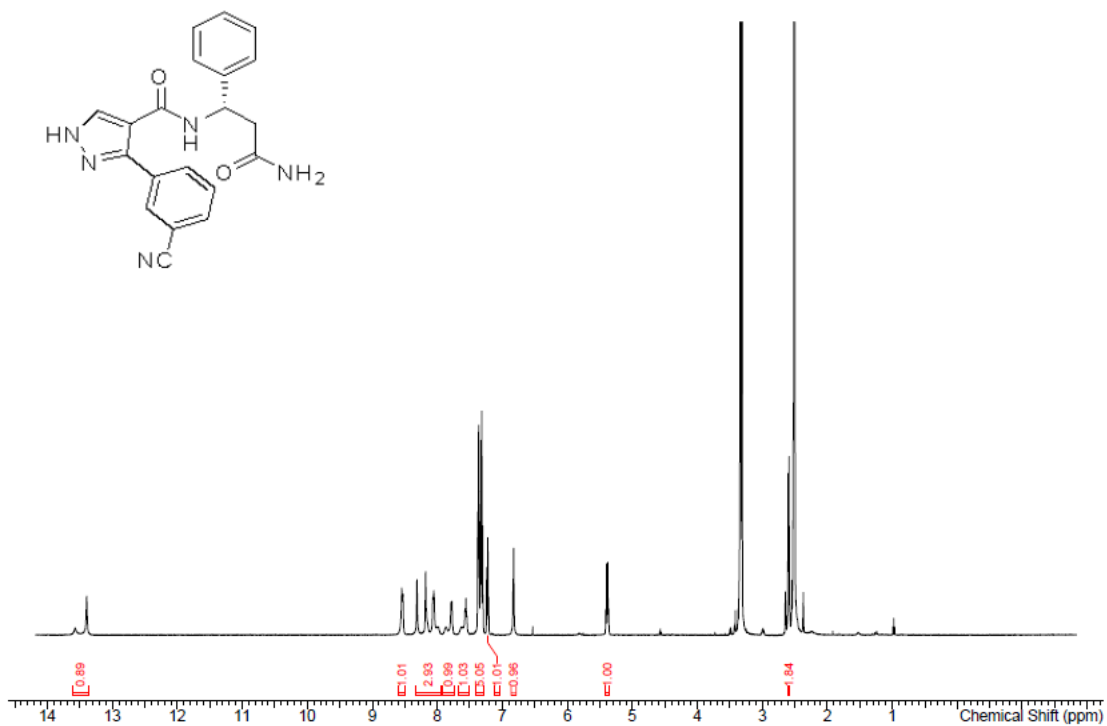
<sup>1</sup>H NMR Spectra for compound **15h** (DMSO-*d*<sub>6</sub>, 500 MHz)

<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz) δ 13.27-13.03 (m, 1H), 8.41-8.34 (m, 1H), 8.18-7.88 (m, 1H), 7.69-7.59 (m, 2H), 7.38-7.28 (m, 5H), 7.25-7.19 (m, 1H), 7.00-6.81 (m, 3H), 5.36 (q, 1H, *J*=7.6 Hz), 3.78 (br d, 3H, *J*=10.0 Hz), 2.57 (br d, 2H, *J*=6.8 Hz)



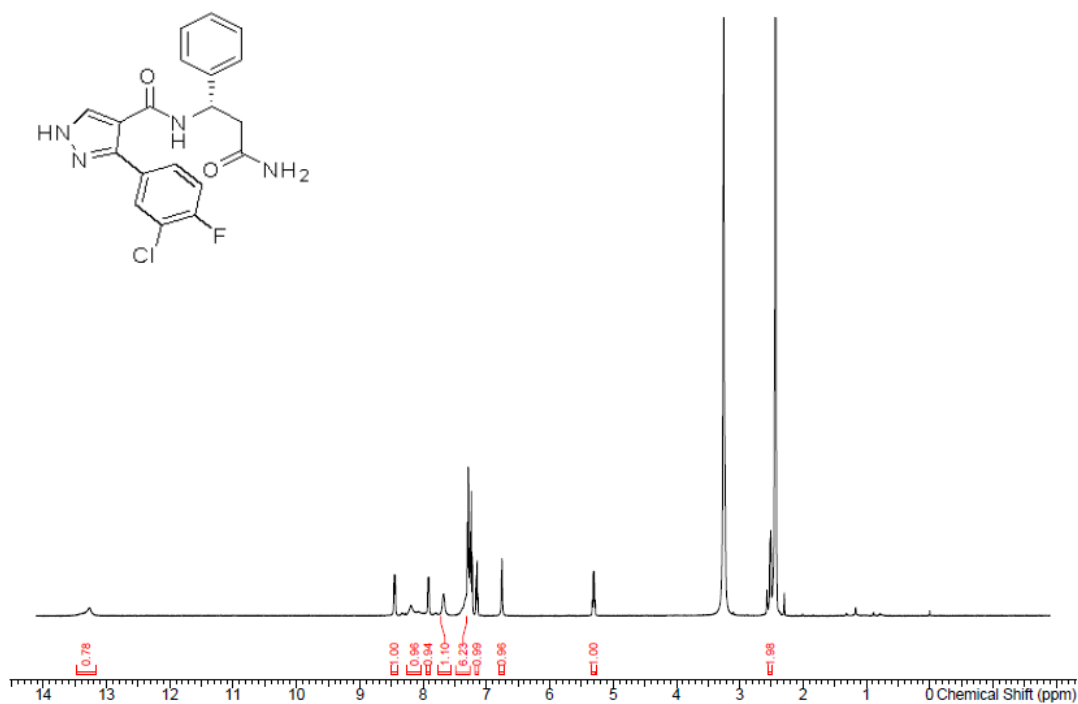
### $^1\text{H}$ NMR Spectra for compound **15i** (DMSO- $d_6$ , 500 MHz)

$^1\text{H}$  NMR (DMSO- $d_6$ , 500 MHz)  $\delta$  13.61-13.36 (m, 1H), 8.54 (br d, 1H,  $J=7.8$  Hz), 8.33-7.95 (m, 3H), 7.92-7.74 (m, 1H), 7.67-7.52 (m, 1H), 7.41-7.29 (m, 5H), 7.26-7.20 (m, 1H), 6.83 (br s, 1H), 5.39 (q, 1H,  $J=7.6$  Hz), 2.59 (br d, 2H,  $J=7.2$  Hz)



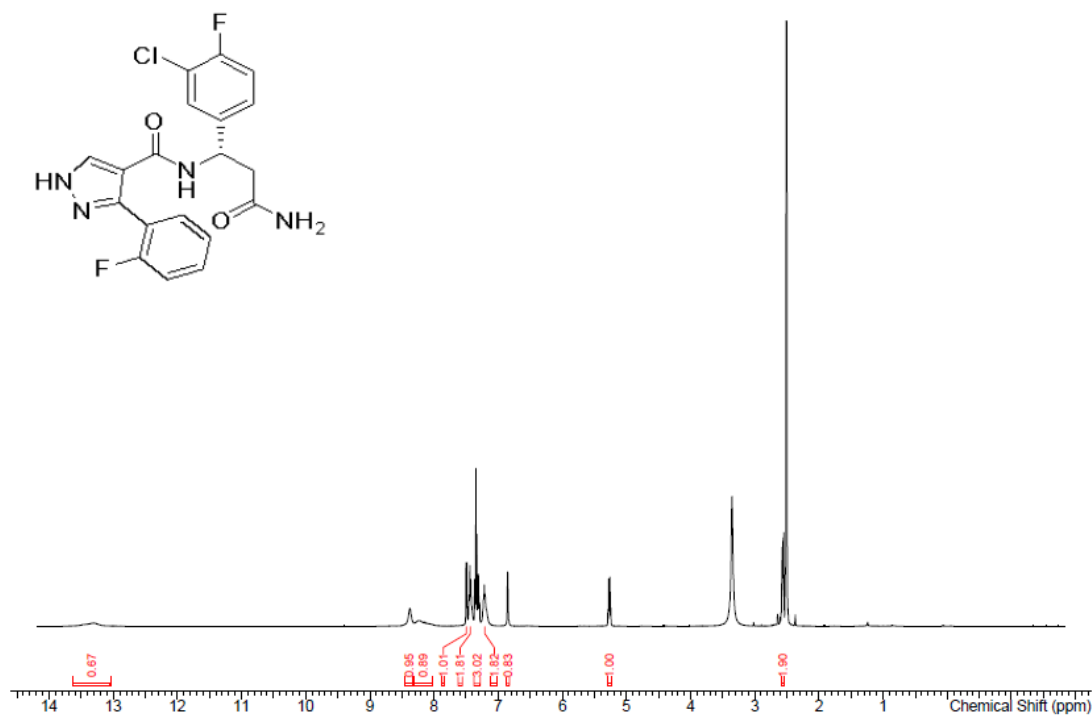
### $^1\text{H}$ NMR Spectra for compound **15j** (DMSO- $d_6$ , 500 MHz)

$^1\text{H}$  NMR (DMSO- $d_6$ , 500 MHz)  $\delta$  13.31 (br s, 1H), 8.45 (br d, 1H,  $J=8.2$  Hz), 8.25-8.02 (m, 1H), 7.91 (br d, 1H,  $J=6.8$  Hz), 7.83-7.61 (m, 1H), 7.42-7.20 (m, 6H), 7.18-7.13 (m, 1H), 6.76 (br s, 1H), 5.31 (q, 1H,  $J=7.4$  Hz), 2.51 (br d, 2H,  $J=6.1$  Hz)



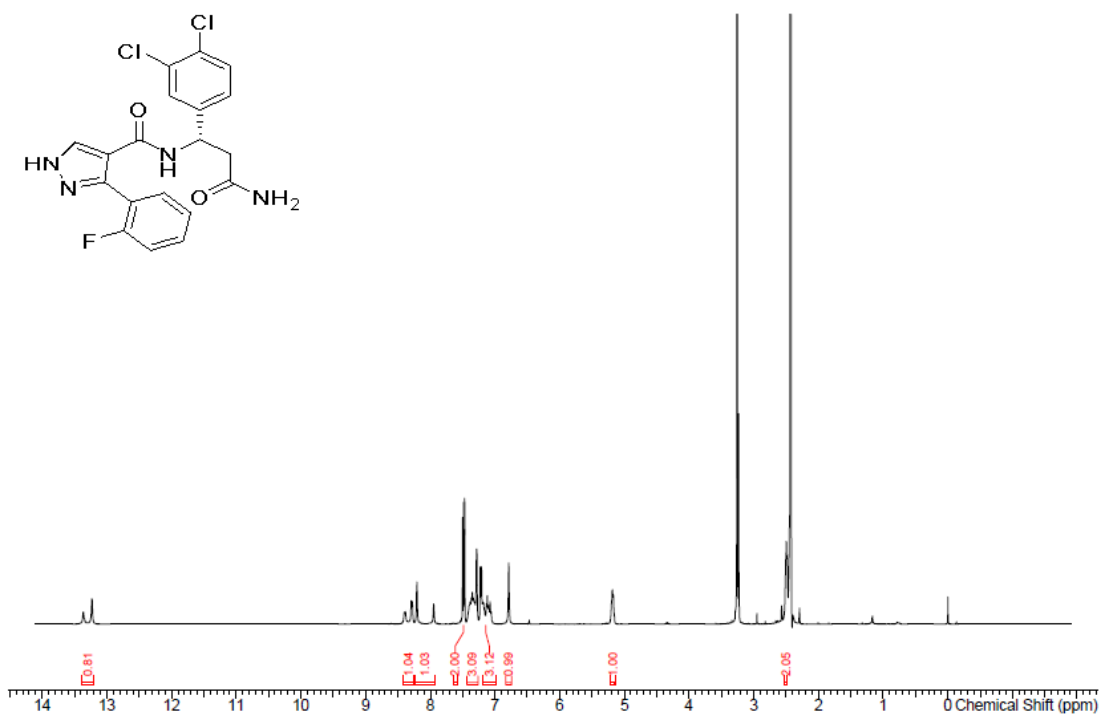
<sup>1</sup>H NMR Spectra for compound **26a** (DMSO-*d*<sub>6</sub>, 500 MHz)

<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz) δ 13.64-13.04 (m, 1H), 8.38 (br s, 1H), 8.14 (br s, 1H), 7.49 (dd, 1H, *J*=2.0, 7.2 Hz), 7.47-7.40 (m, 2H), 7.38-7.28 (m, 3H), 7.26-7.16 (m, 2H), 6.85 (br s, 1H), 5.27 (q, 1H, *J*=7.5 Hz), 2.57 (br dd, 2H, *J*=1.9, 7.3 Hz)



<sup>1</sup>H NMR Spectra for compound **26b** (DMSO-*d*<sub>6</sub>, 500 MHz)

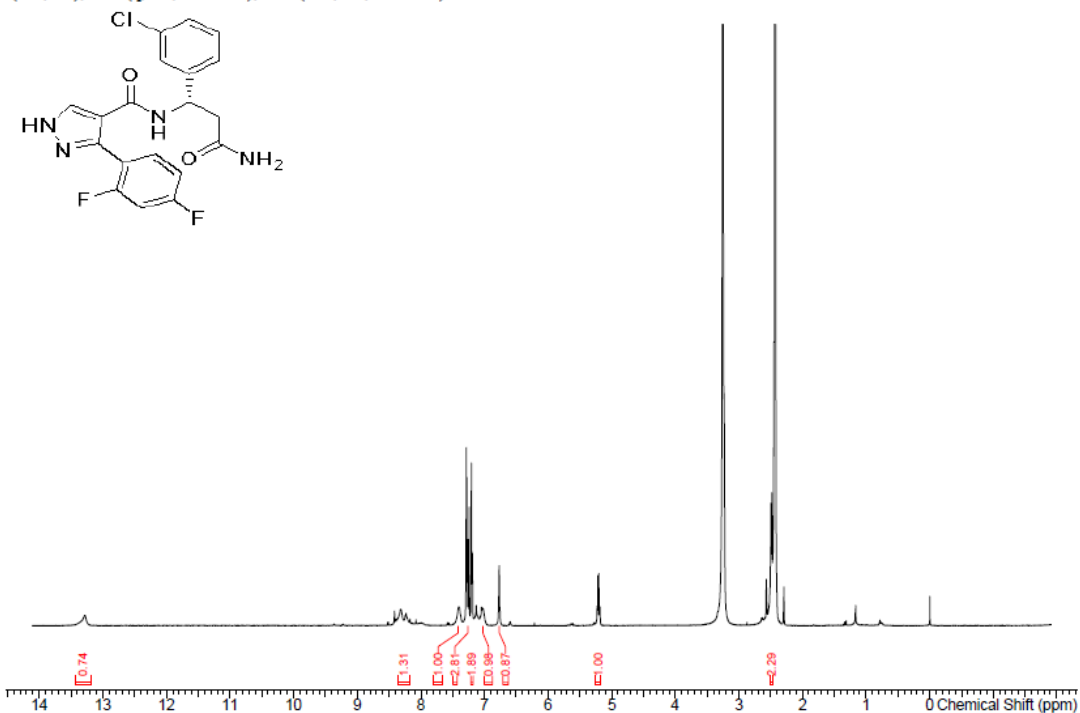
<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz) δ 13.39-13.20 (m, 1H), 8.42-8.26 (m, 1H), 8.24-7.92 (m, 1H), 7.51-7.46 (m, 2H), 7.43-7.26 (m, 3H), 7.24-7.04 (m, 3H), 6.79 (br s, 1H), 5.21-5.15 (m, 1H), 2.49 (br d, 2H, *J*=6.2 Hz)





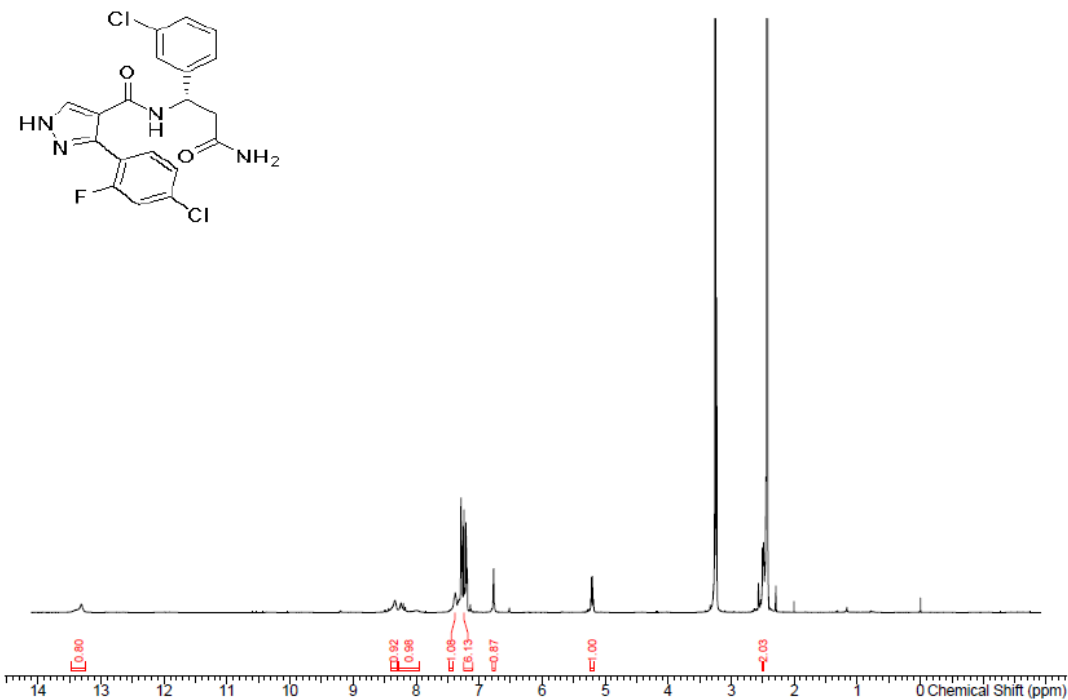
### <sup>1</sup>H NMR Spectra for compound **26c** (DMSO-*d*<sub>6</sub>, 500 MHz)

<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz) δ 13.32 (br s, 1H), 8.36-8.18 (m, 1H), 7.40 (br s, 1H), 7.29-7.23 (m, 3H), 7.22-7.18 (m, 2H), 7.05 (br s, 1H), 6.77 (br s, 1H), 5.21 (q, 1H, *J*=7.4 Hz), 2.49 (br d, 2H, *J*=7.3 Hz)



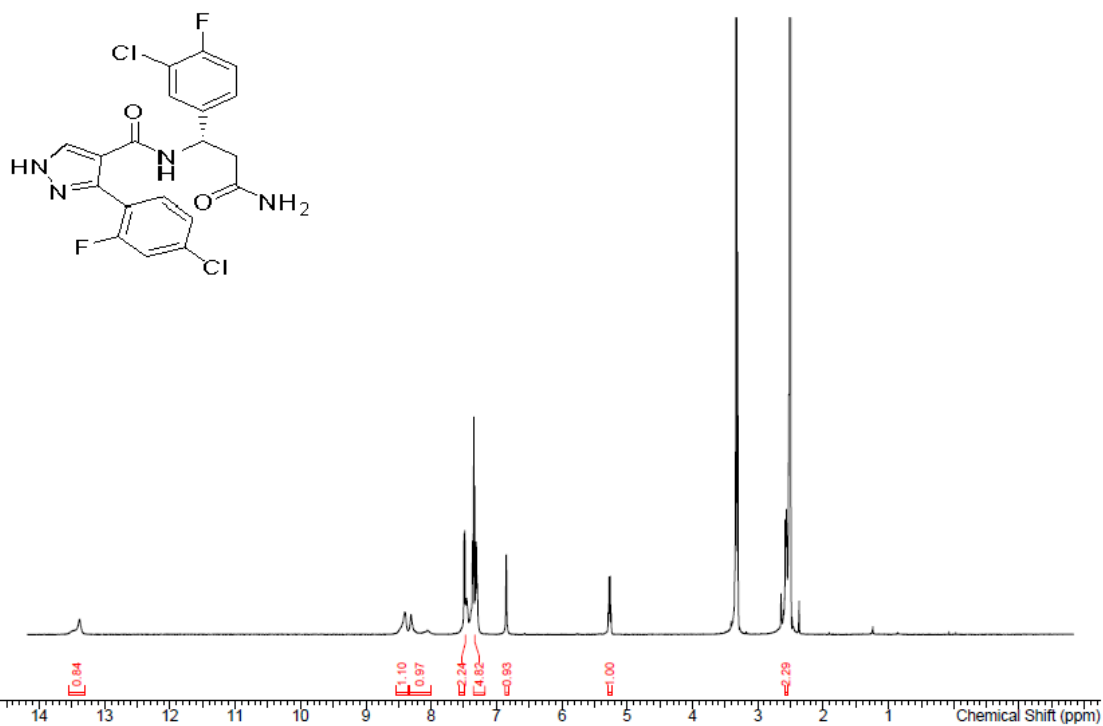
### <sup>1</sup>H NMR Spectra for compound **26d** (DMSO-*d*<sub>6</sub>, 500 MHz)

<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz) δ 13.46-13.24 (m, 1H), 8.33 (br s, 1H), 8.27-7.94 (m, 1H), 7.38 (br s, 1H), 7.31-7.17 (m, 6H), 6.77 (br s, 1H), 5.21 (q, 1H, *J*=7.5 Hz), 2.49 (br dd, 2H, *J*=3.2, 7.3 Hz)

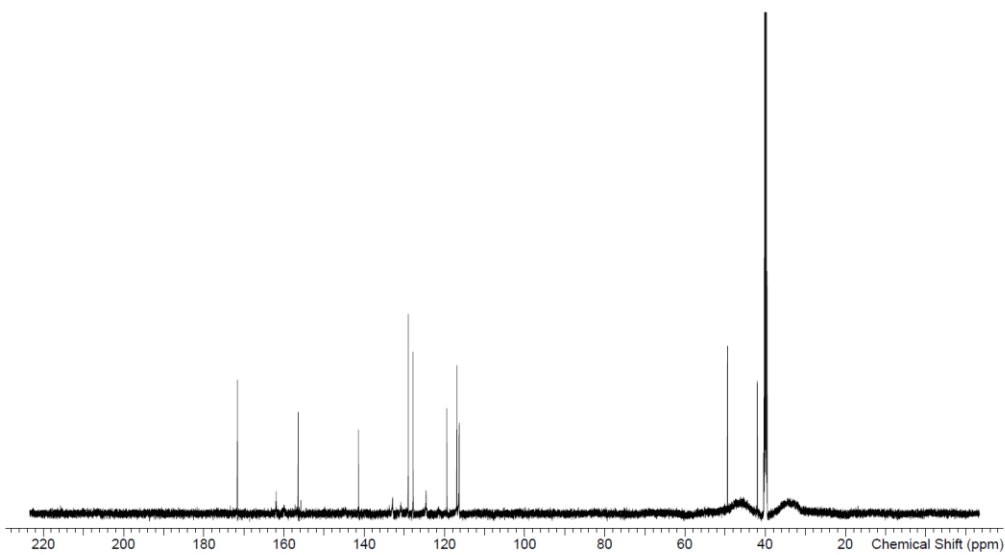


### <sup>1</sup>H NMR Spectra for compound **26e** (DMSO-*d*<sub>6</sub>, 500 MHz)

<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz) δ 13.54-13.30 (m, 1H), 8.40 (br s, 1H), 8.34-8.01 (m, 1H), 7.52-7.43 (m, 2H), 7.42-7.25 (m, 5H), 6.85 (br s, 1H), 5.27 (q, 1H, *J*=7.5 Hz), 2.57 (br dd, 2H, *J*=2.8, 7.2 Hz)



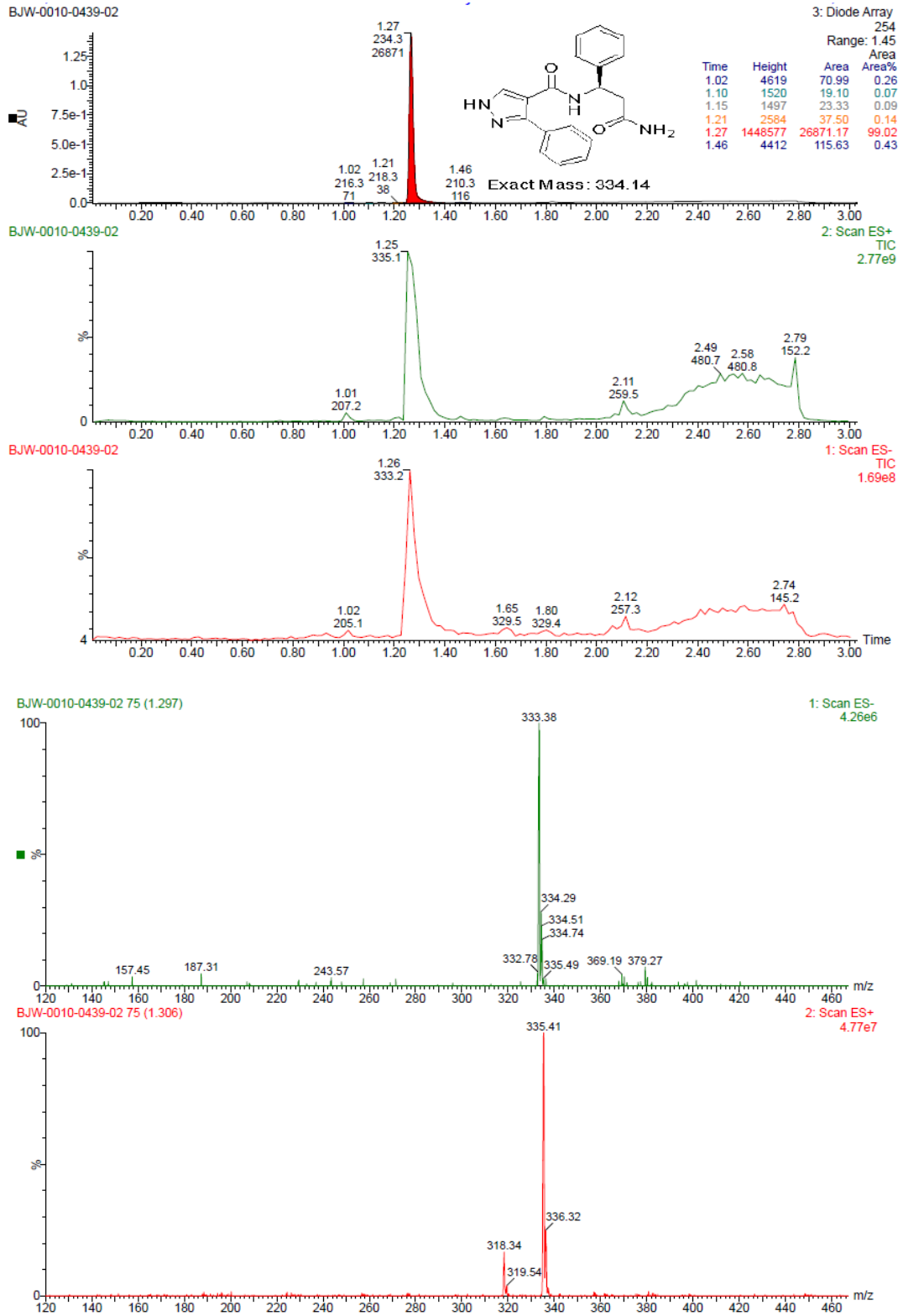
### <sup>13</sup>C NMR Spectra for compound **26e** (DMSO-*d*<sub>6</sub>, 176 MHz)



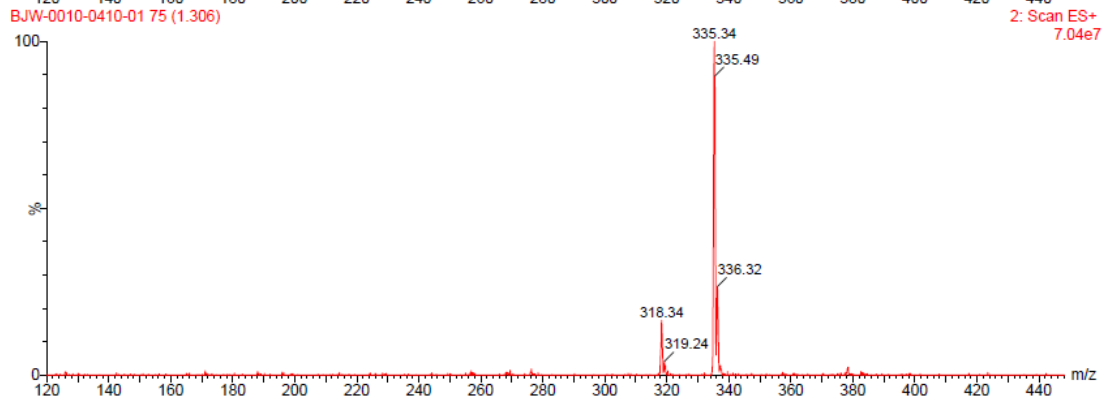
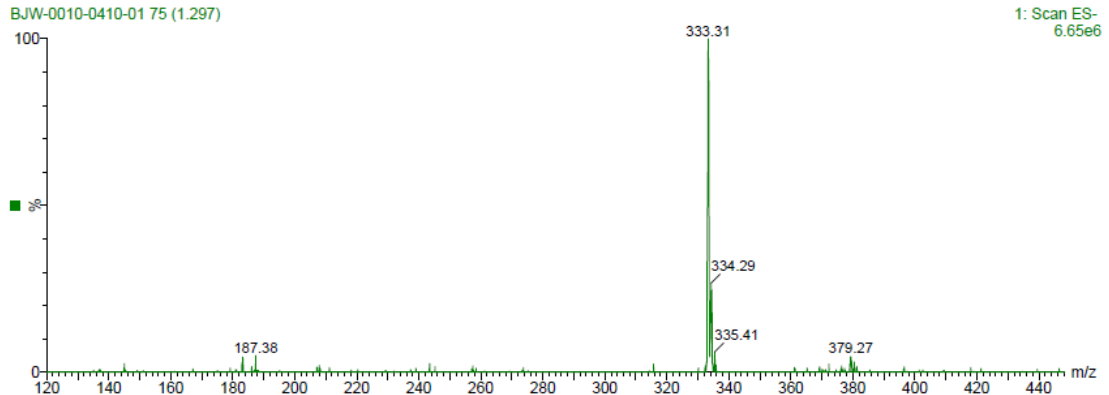
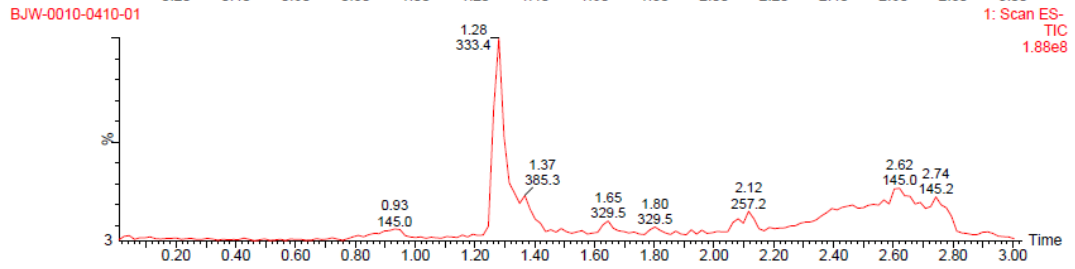
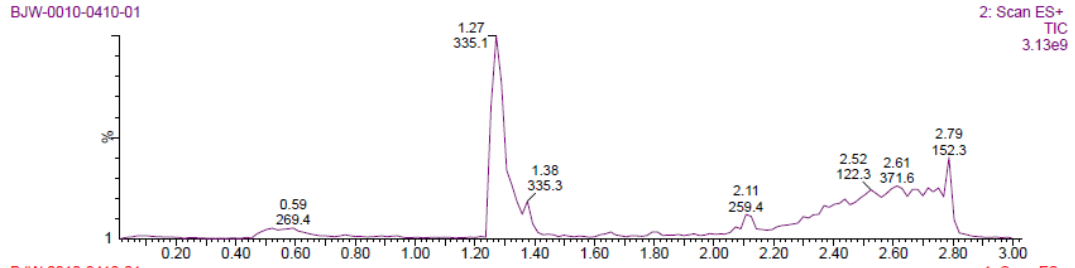
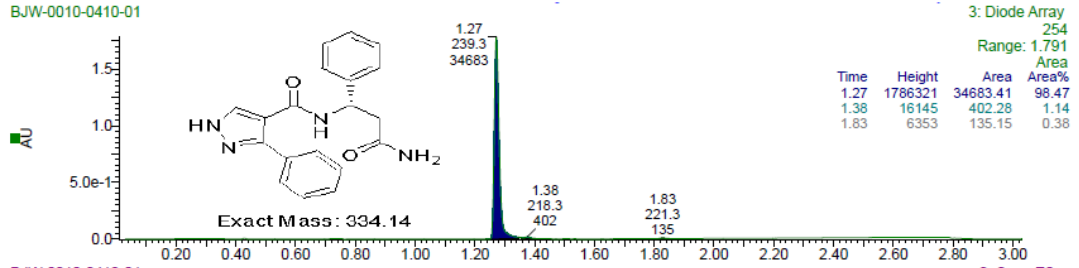
<sup>13</sup>C NMR (176 MHz, DMSO-*d*<sub>6</sub>) δ ppm 171.6, 161.9, 160.0, 155.8, 141.4, 132.9, 130.8, 129.0, 127.8, 124.6, 119.4, 116.9, 116.3, 49.4, 42.0

### 3. LCMS Spectra for tested compounds

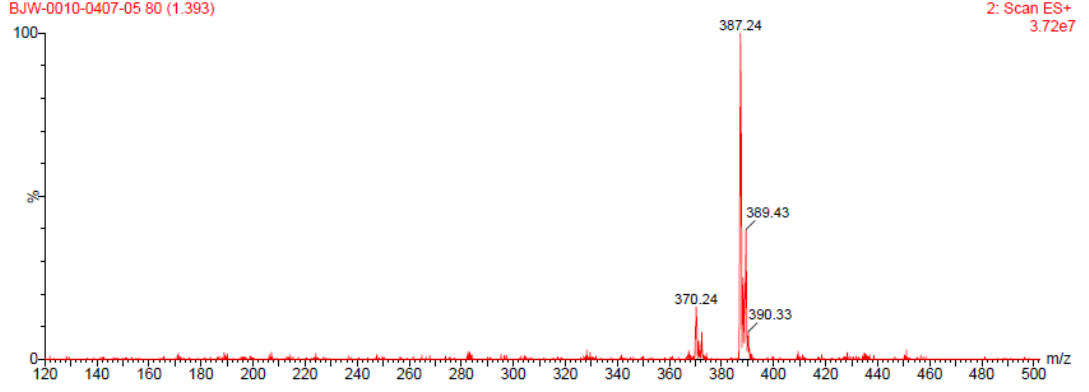
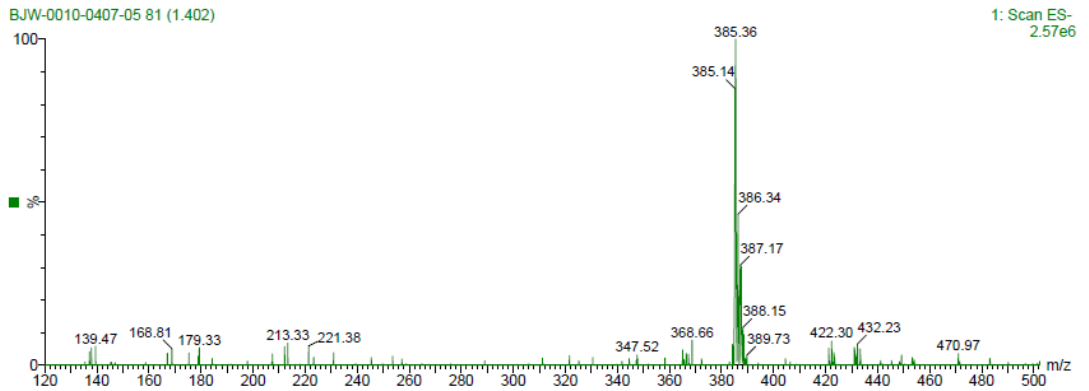
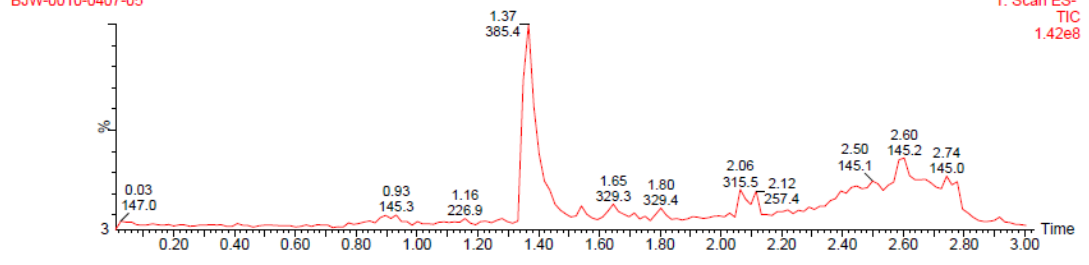
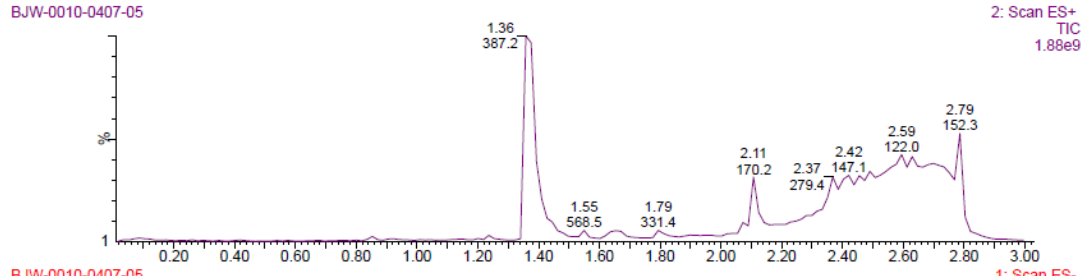
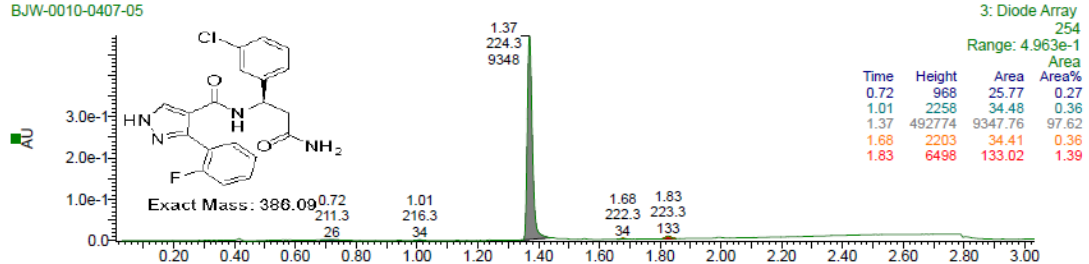
#### LCMS Spectra for compound 3a



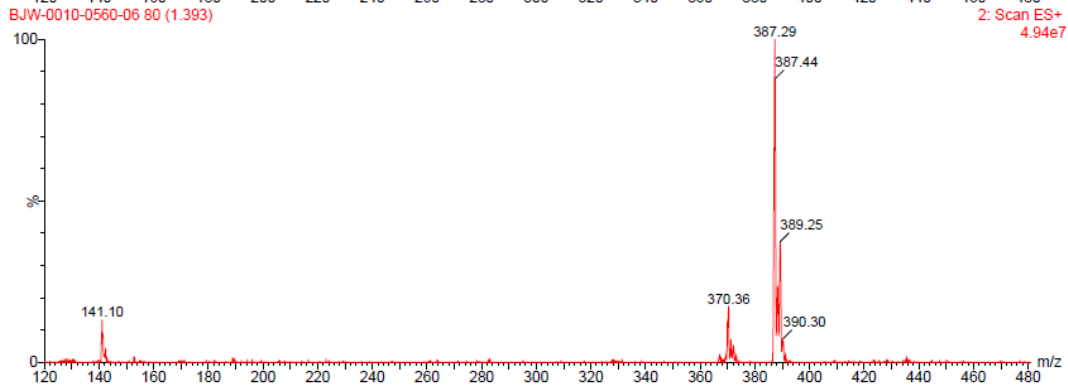
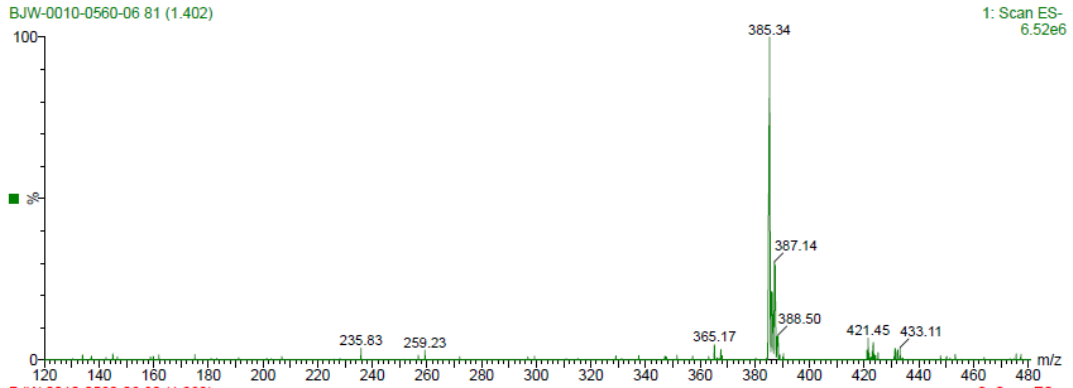
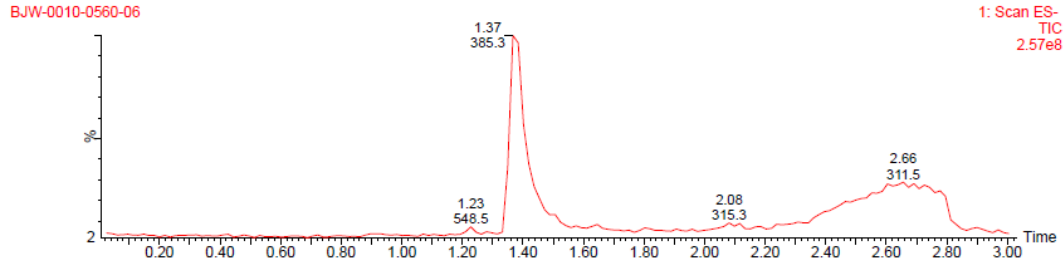
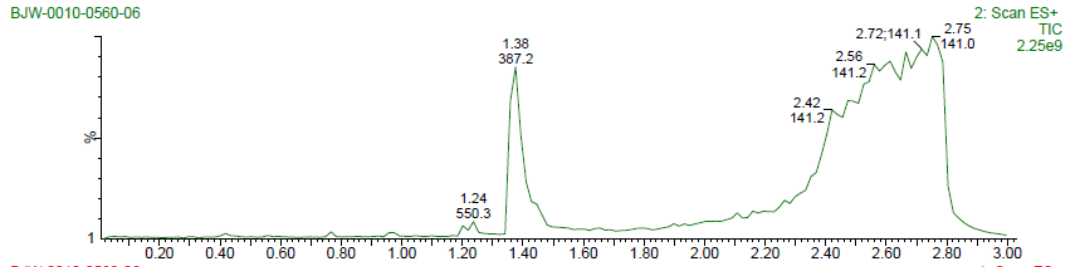
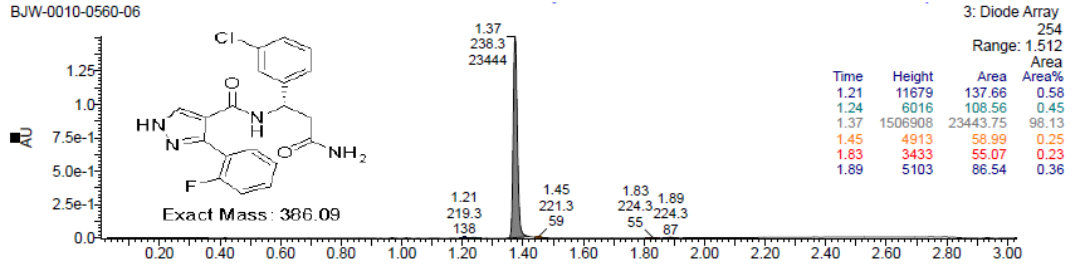
# LCMS Spectra for compound 3b



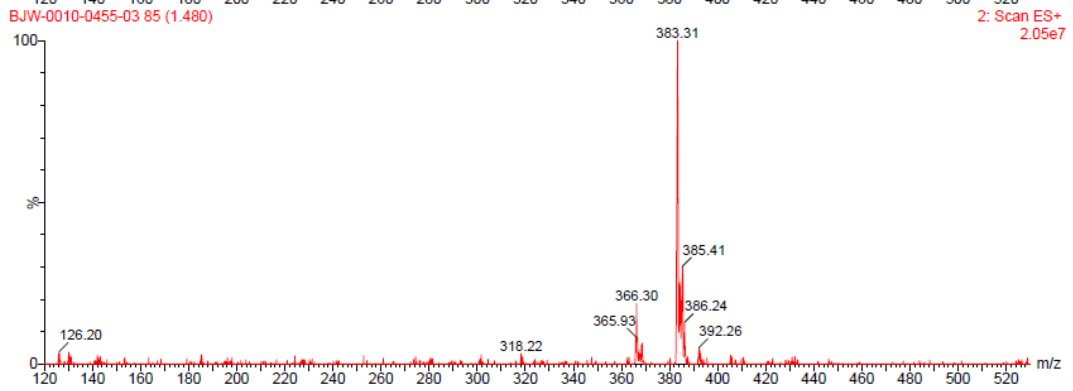
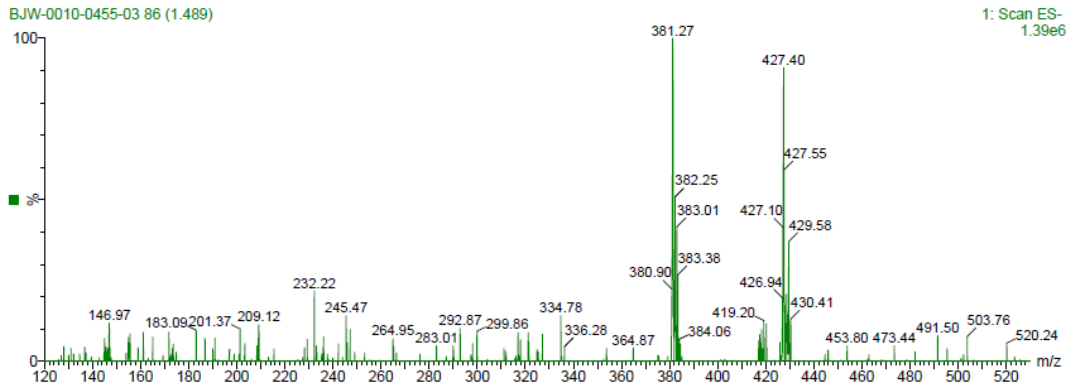
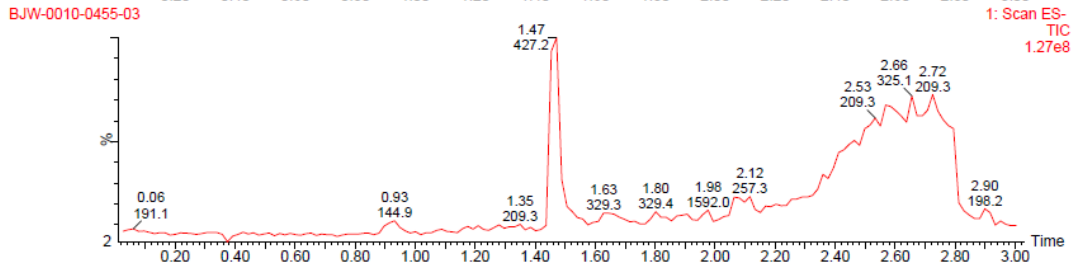
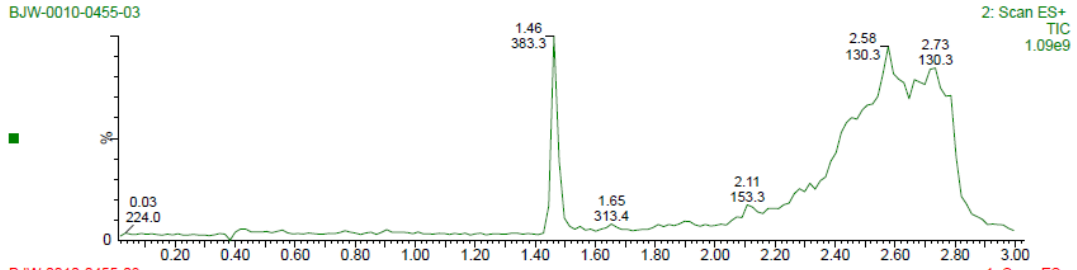
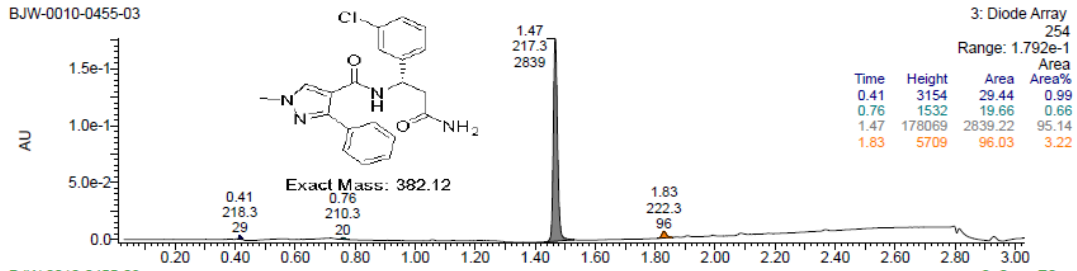
# LCMS Spectra for compound 3c



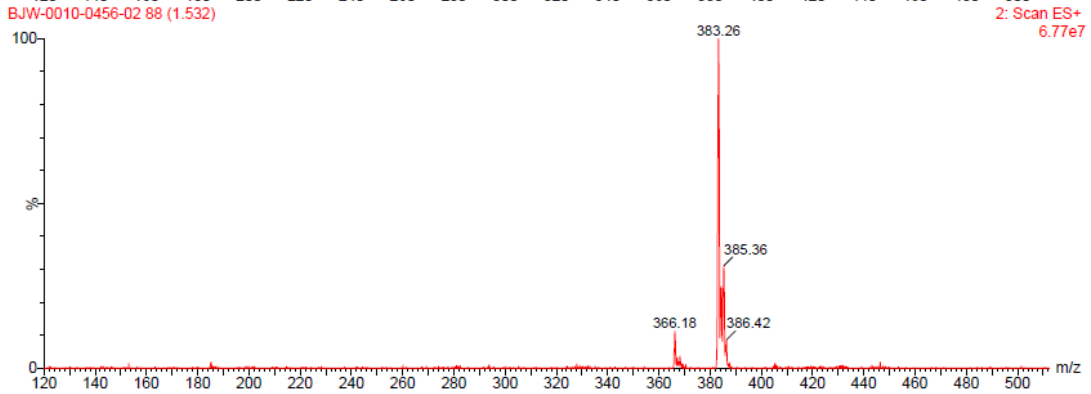
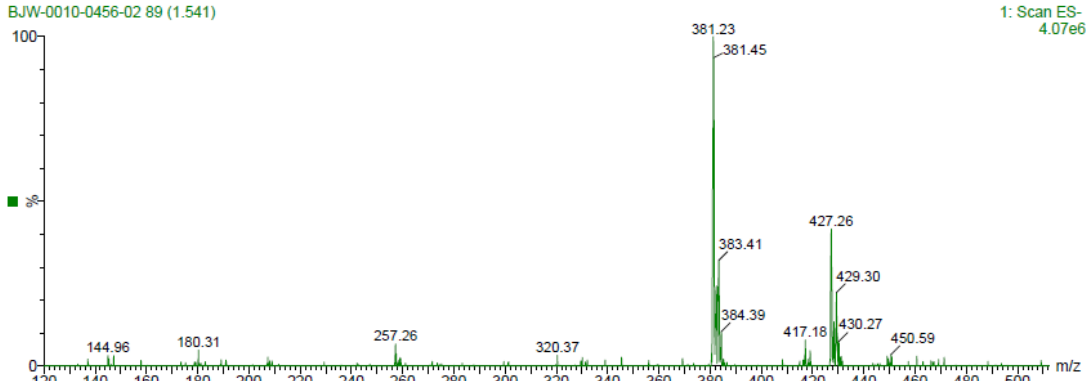
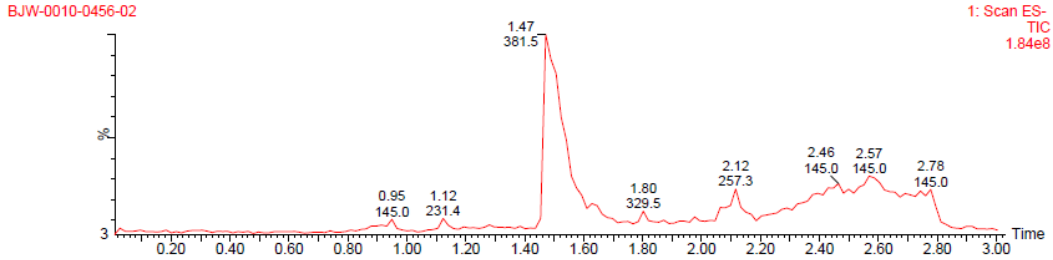
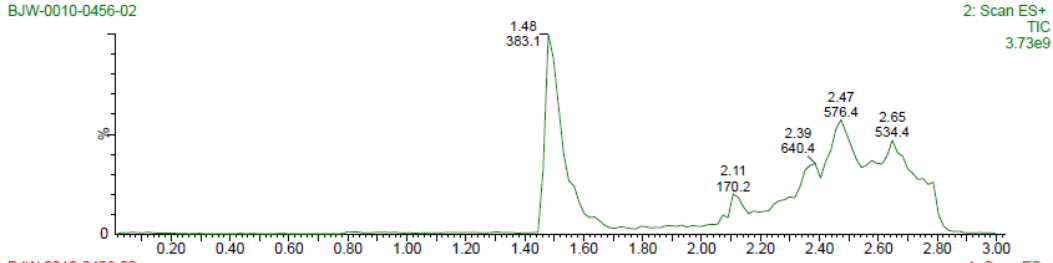
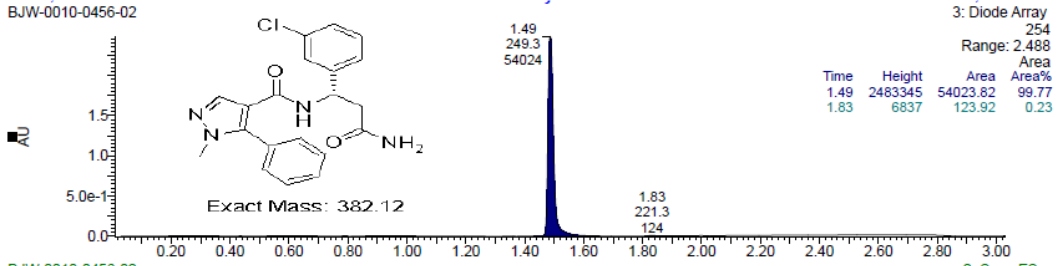
# LCMS Spectra for compound 3d



# LCMS Spectra for compound 5a

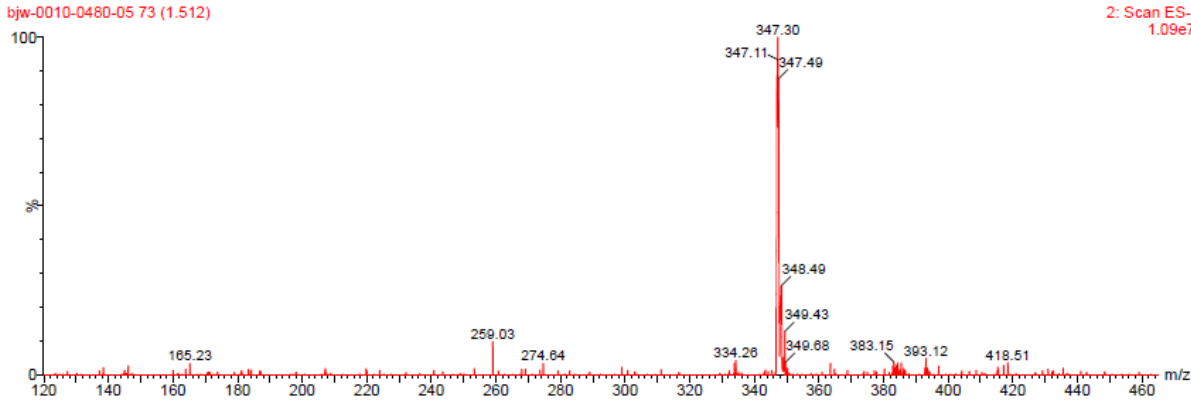
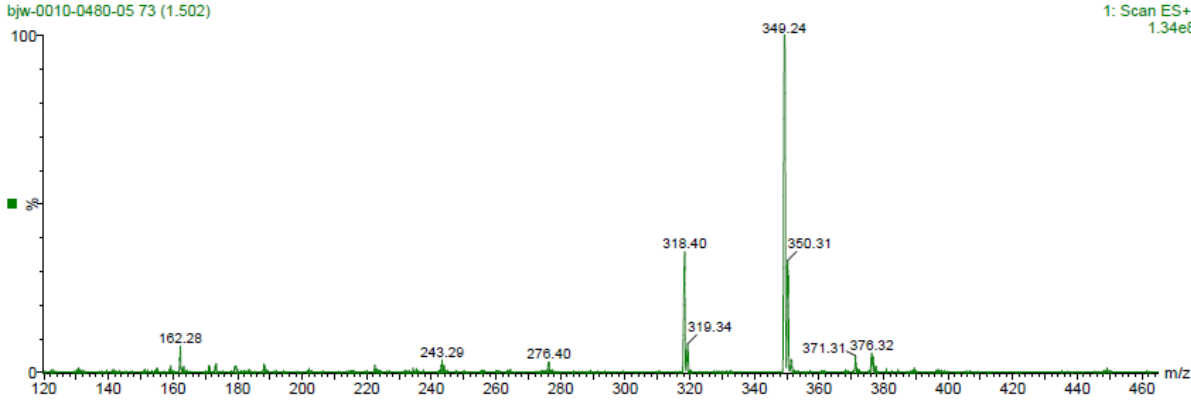
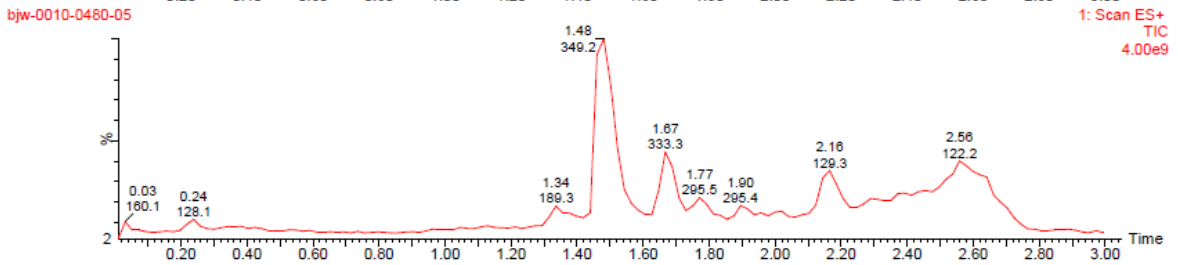
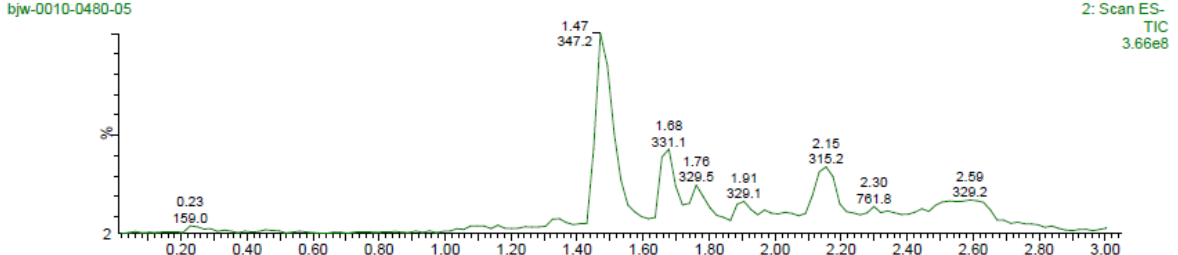
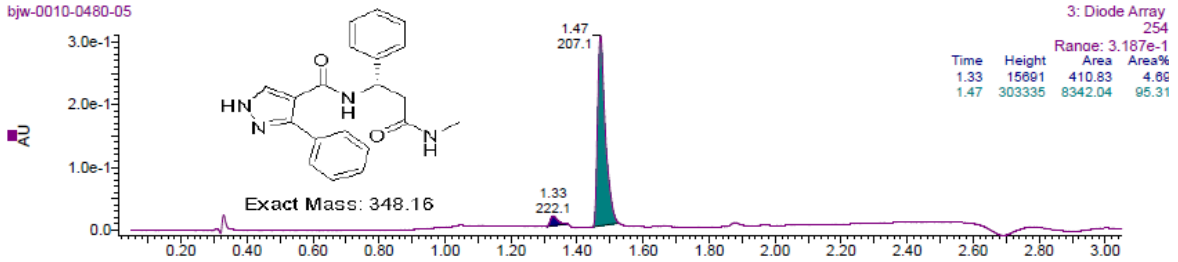


# LCMS Spectra for compound 5b

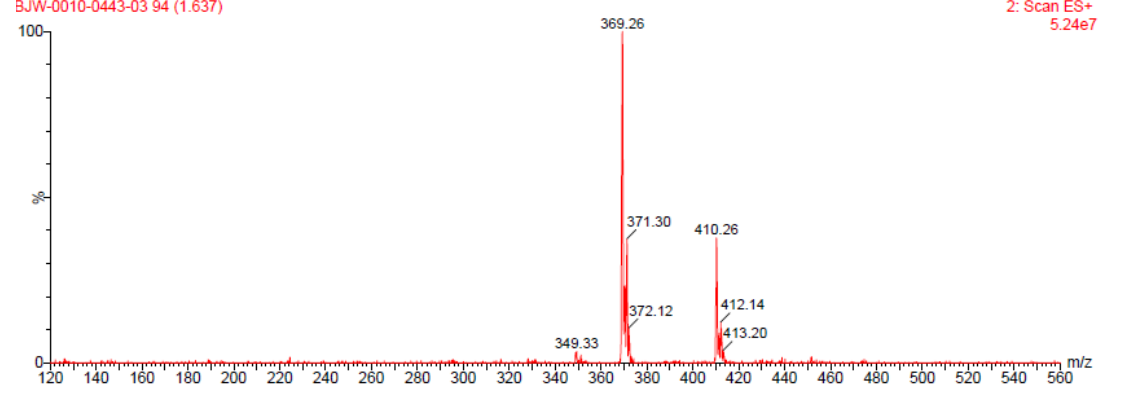
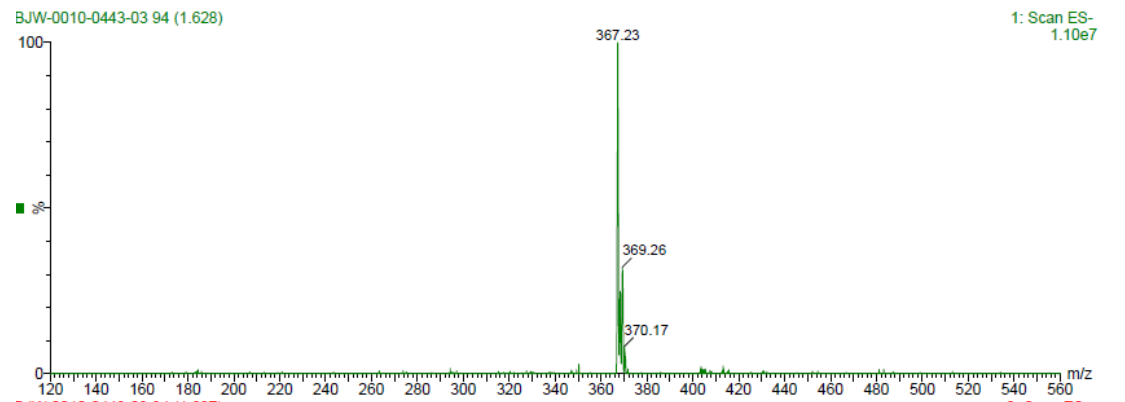
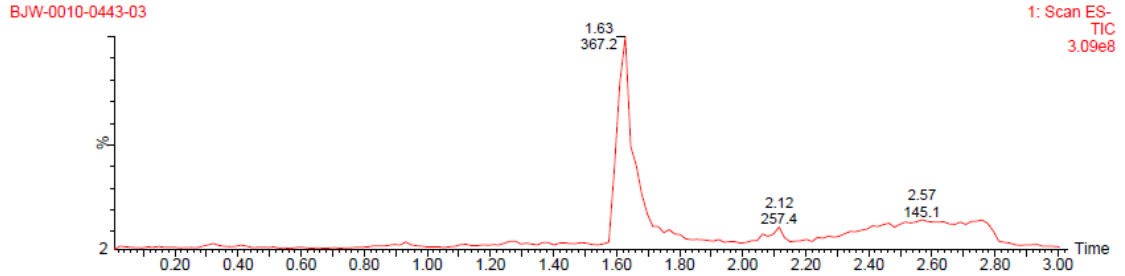
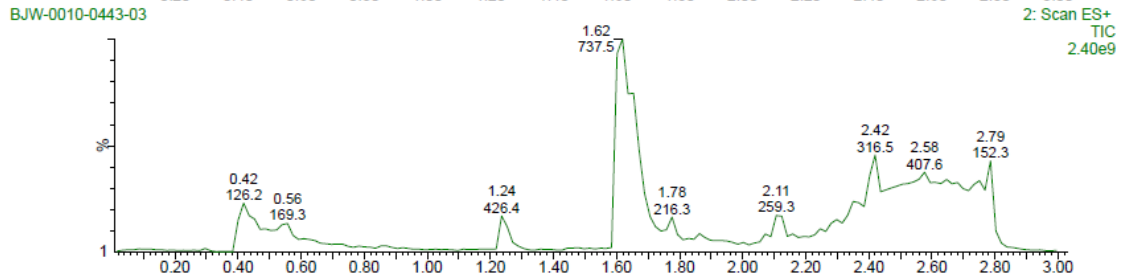
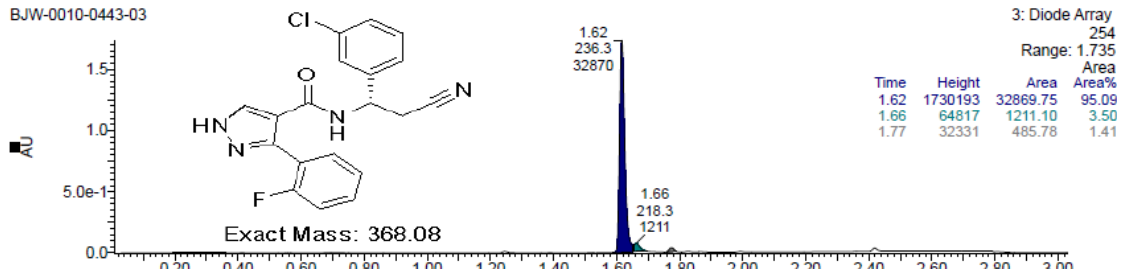




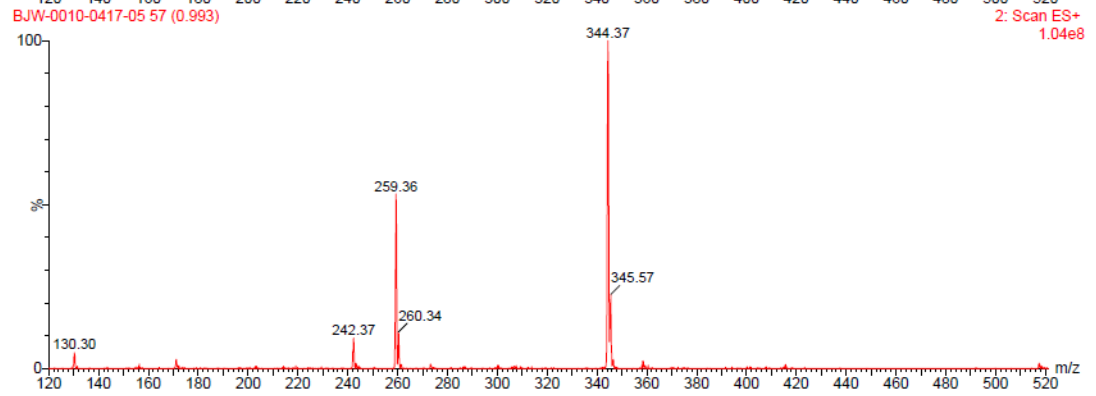
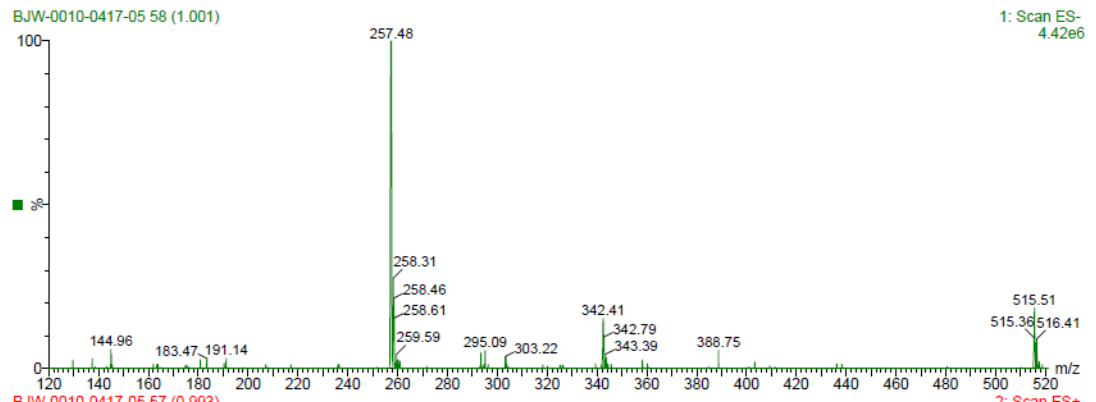
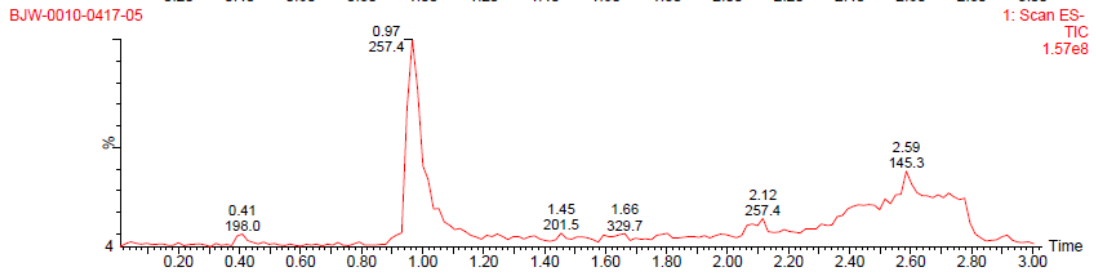
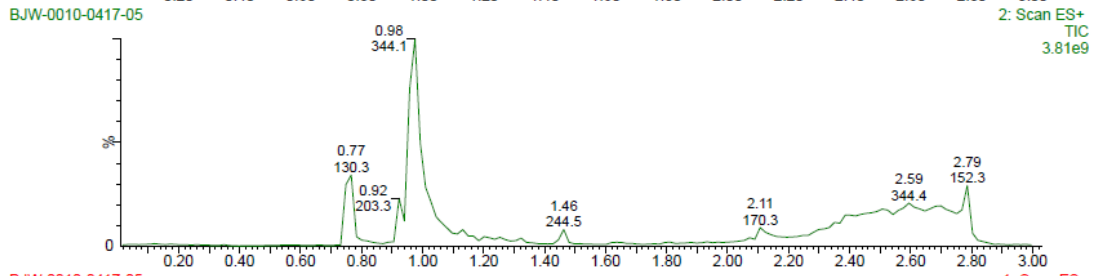
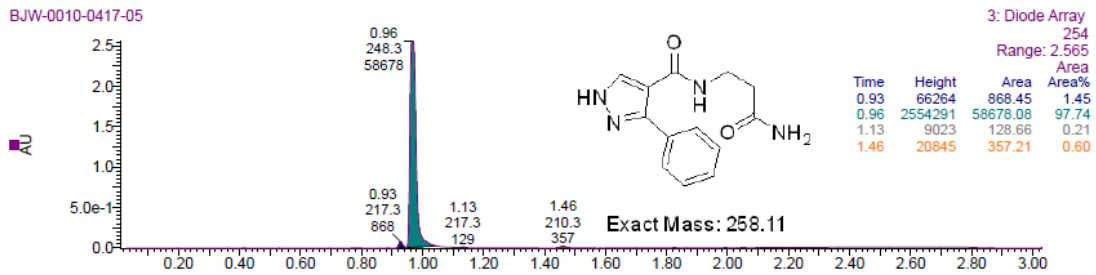
# LCMS Spectra for compound 5c



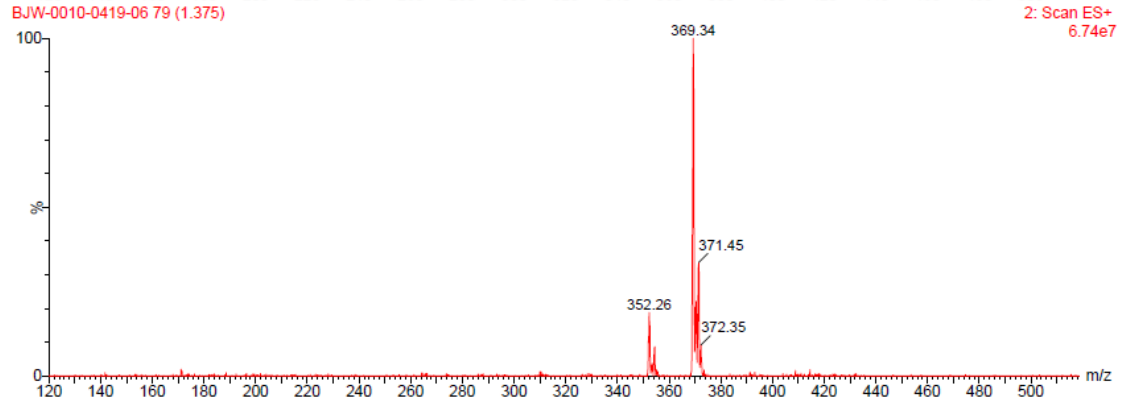
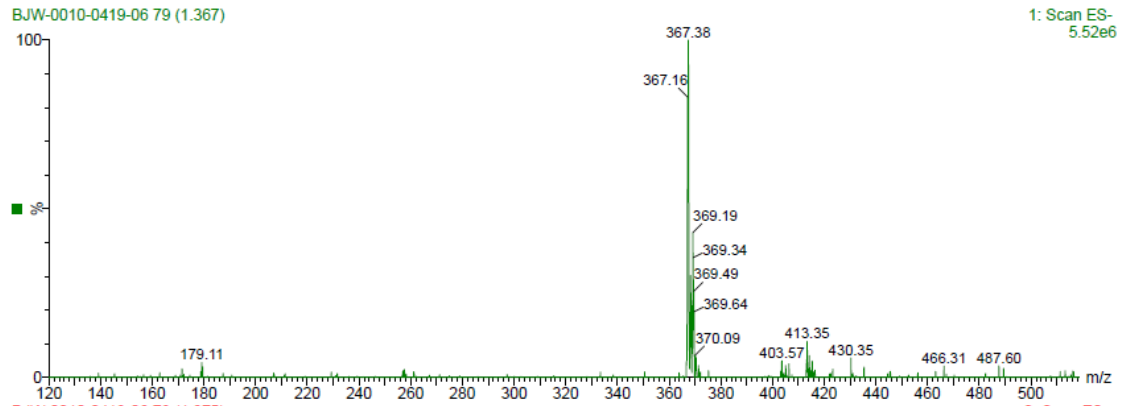
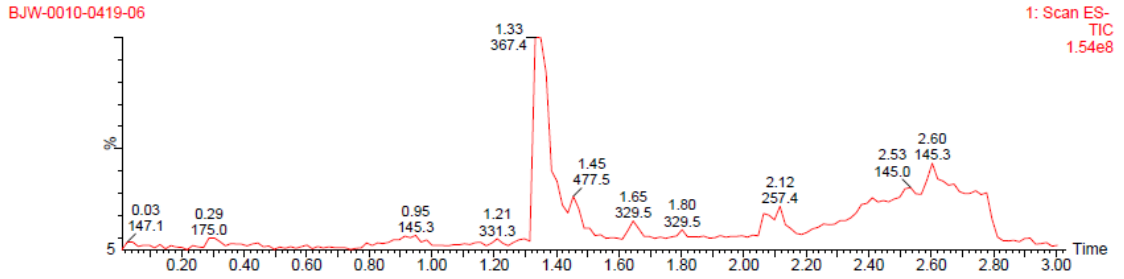
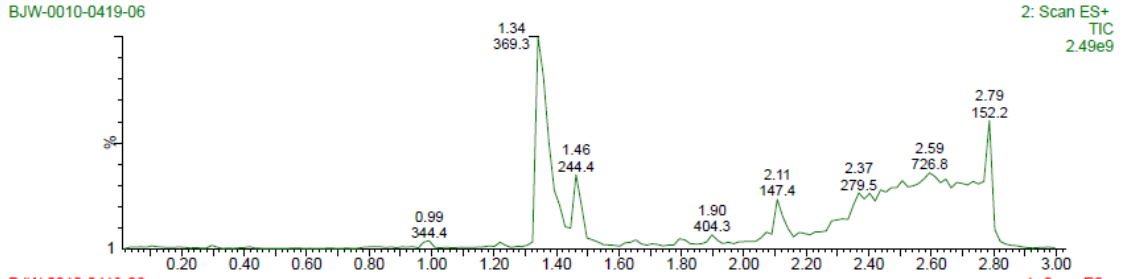
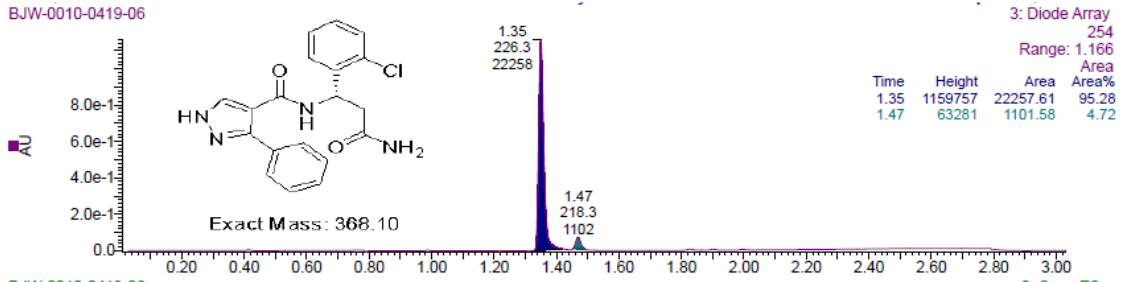
# LCMS Spectra for compound 5d



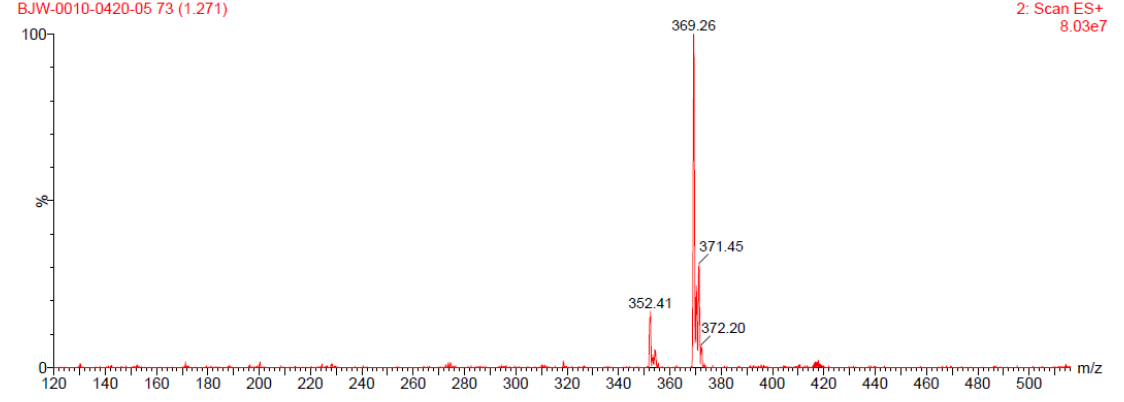
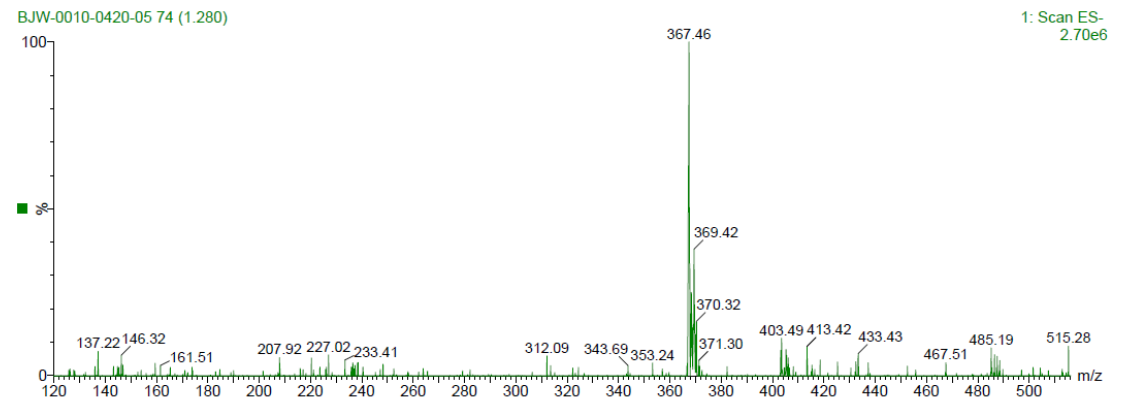
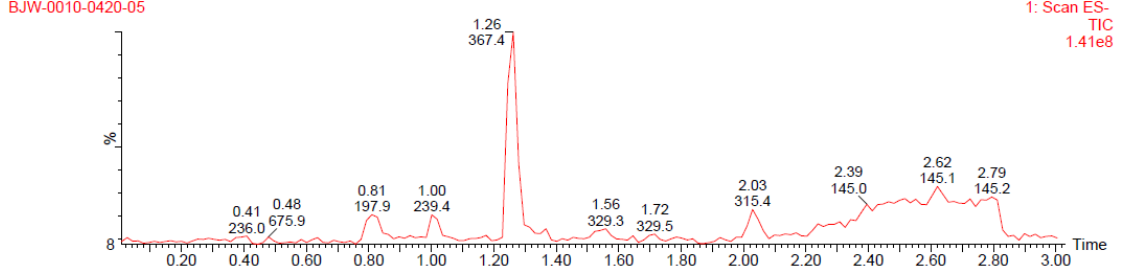
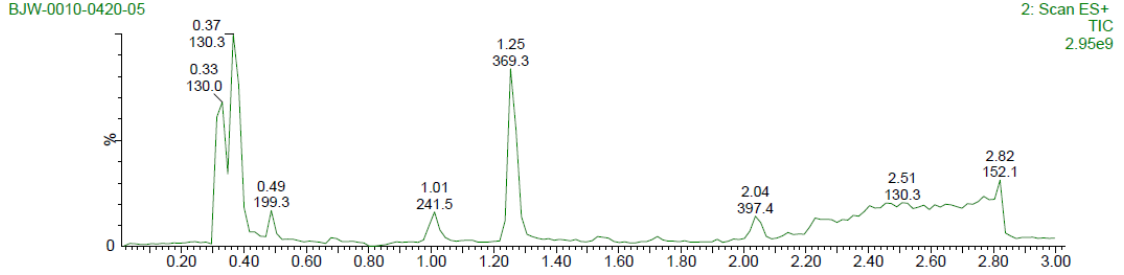
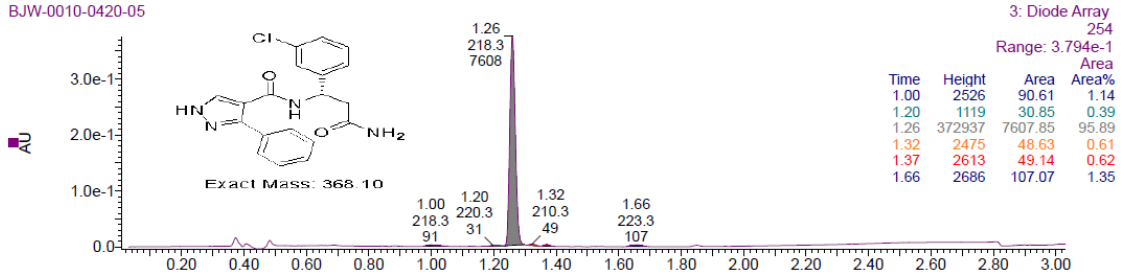
# LCMS Spectra for compound 14a



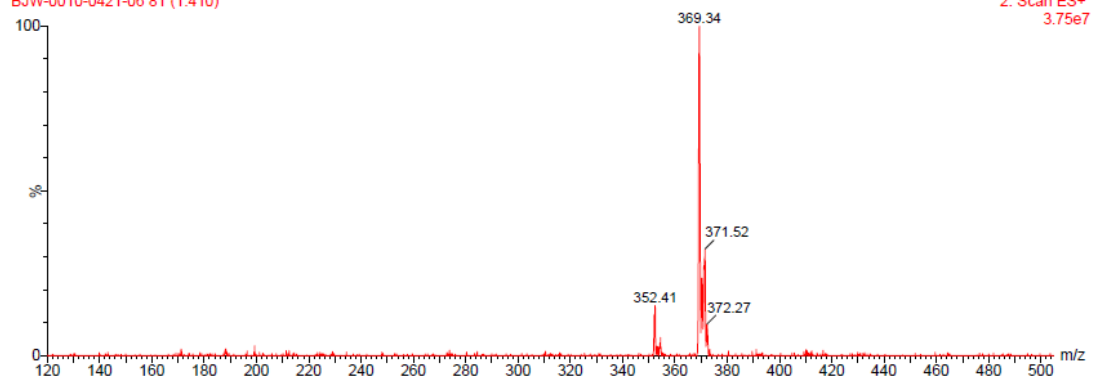
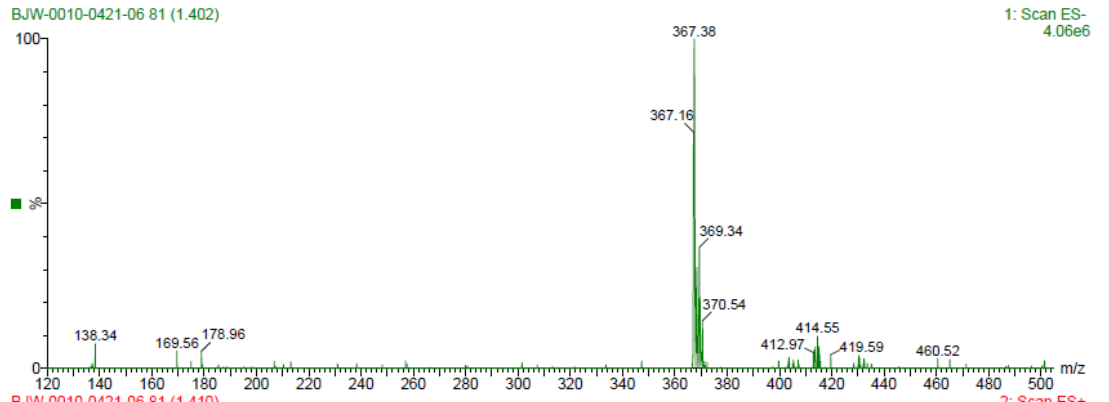
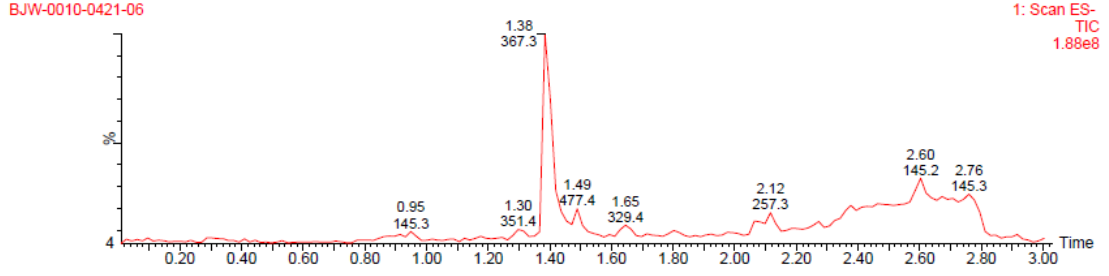
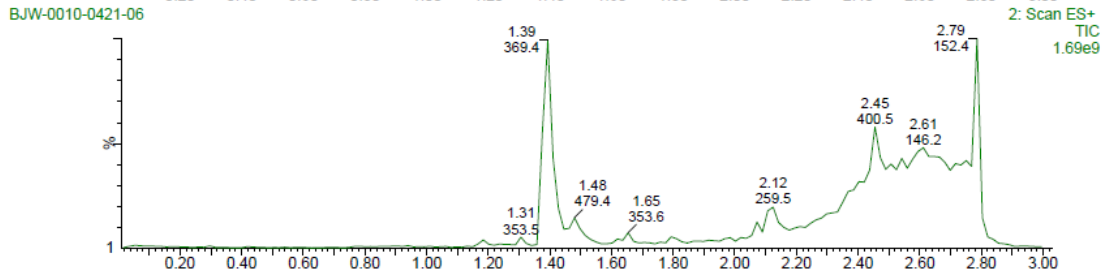
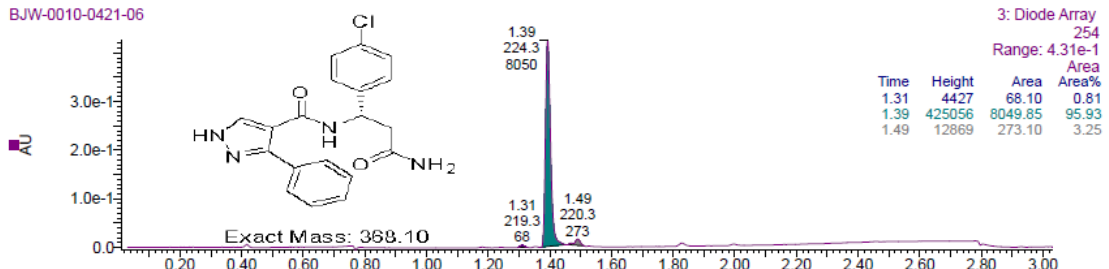
# LCMS Spectra for compound 14b



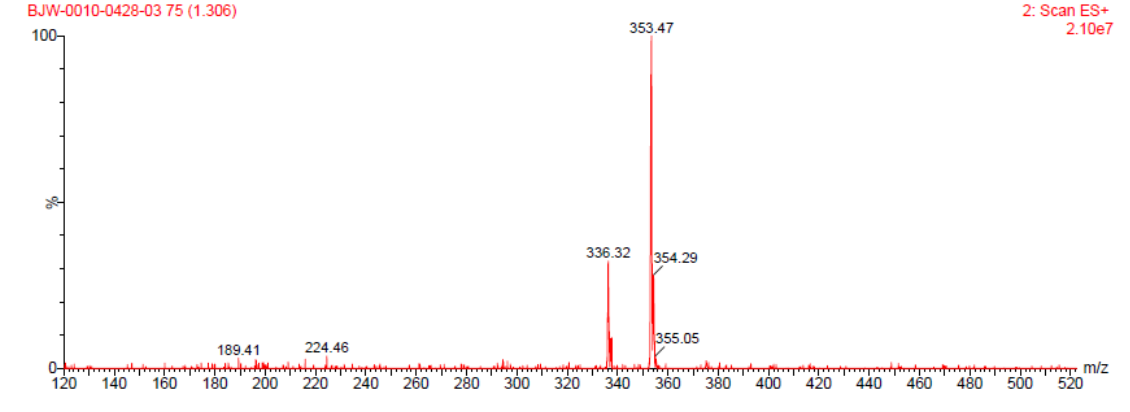
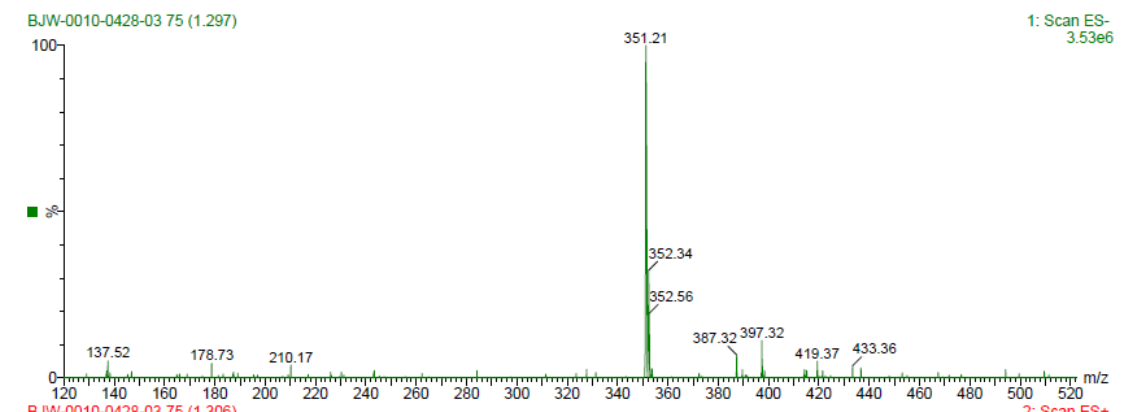
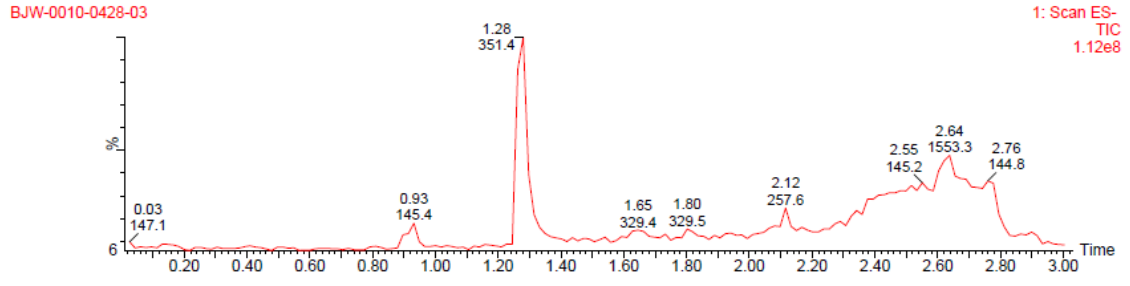
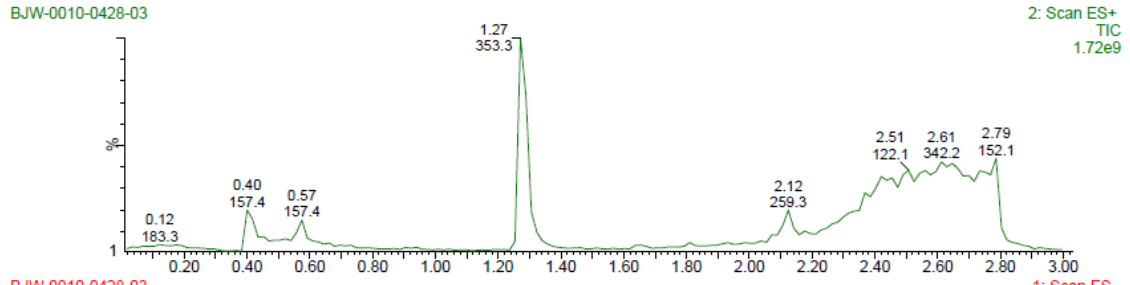
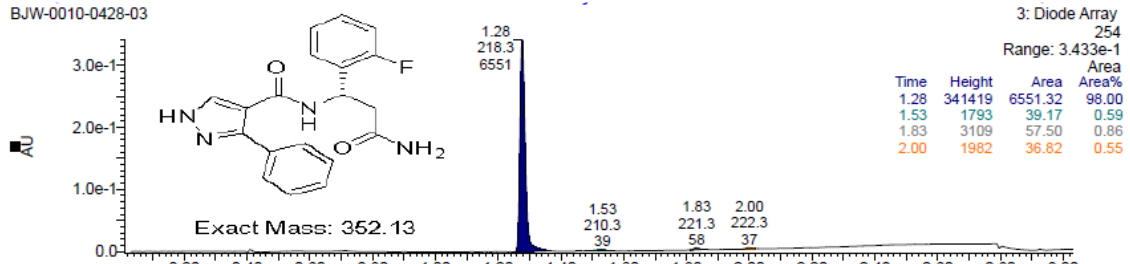
# LCMS Spectra for compound 14c



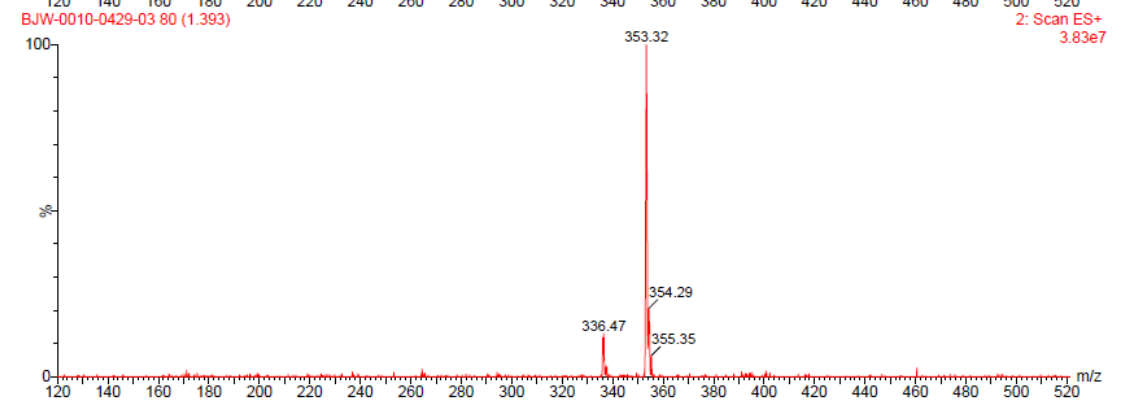
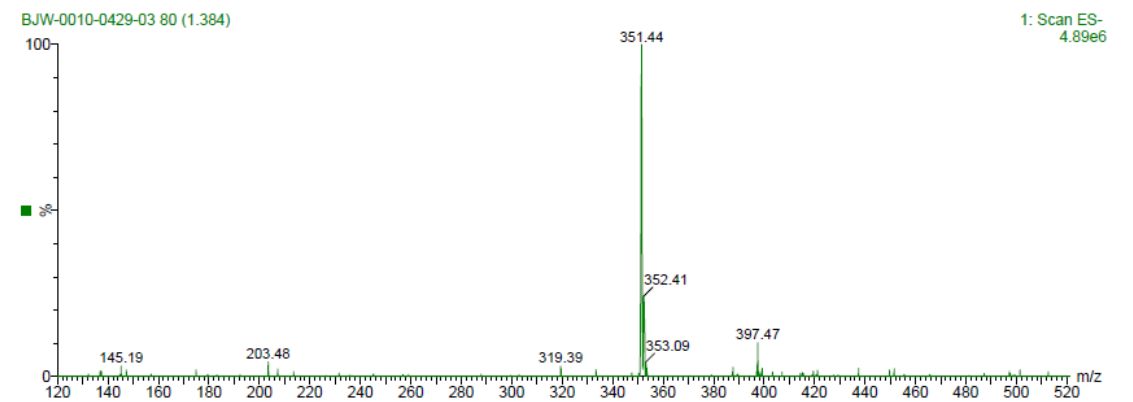
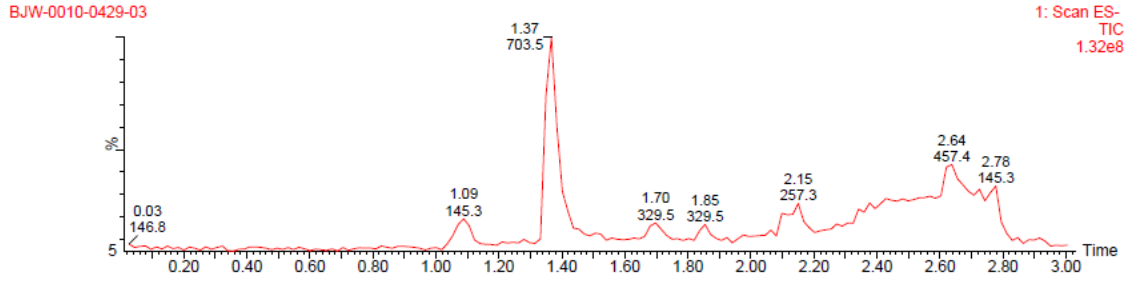
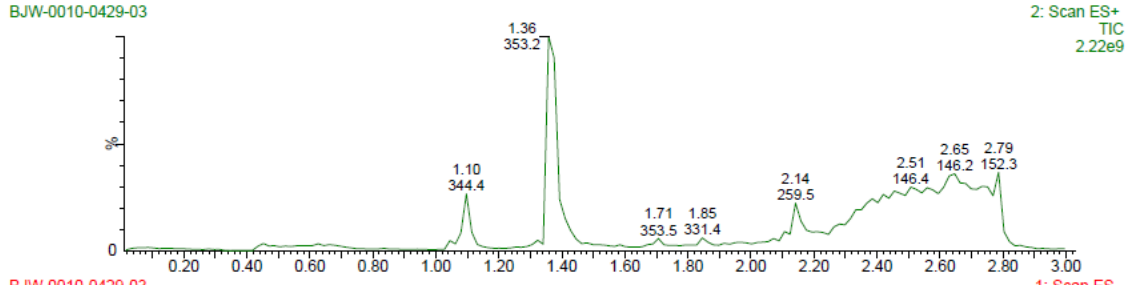
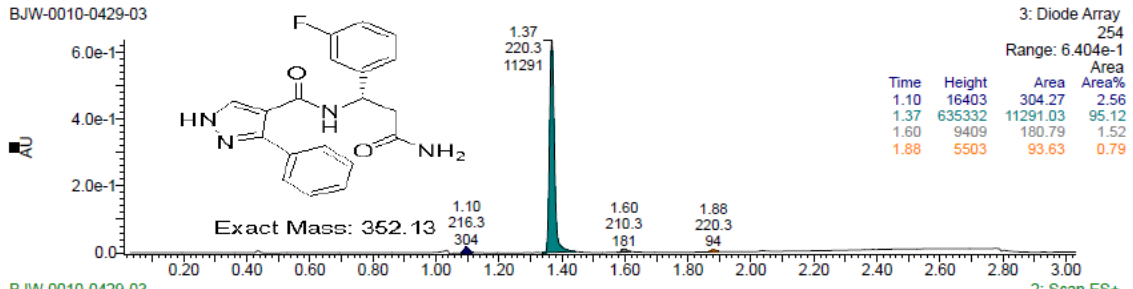
# LCMS Spectra for compound 14d



# LCMS Spectra for compound 14e

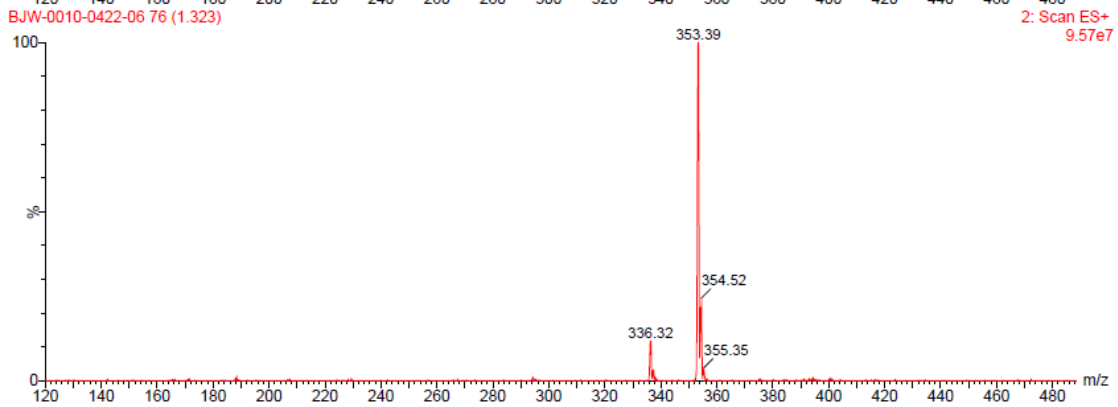
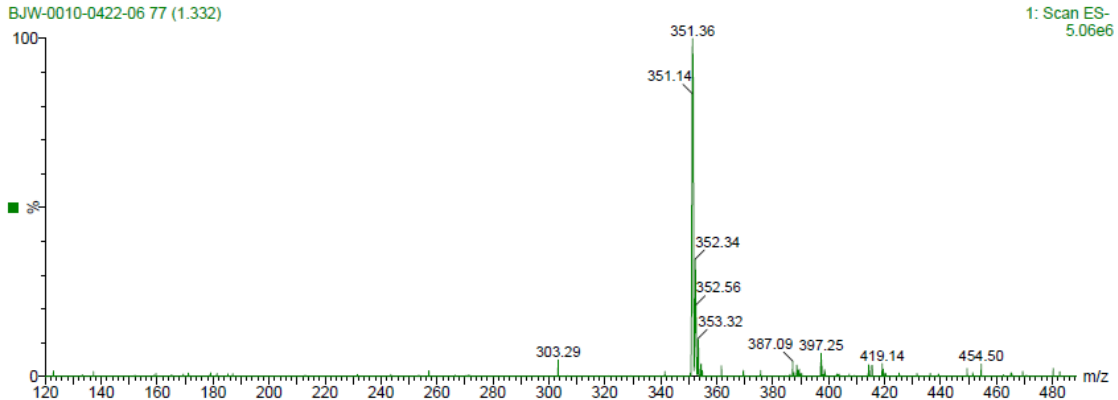
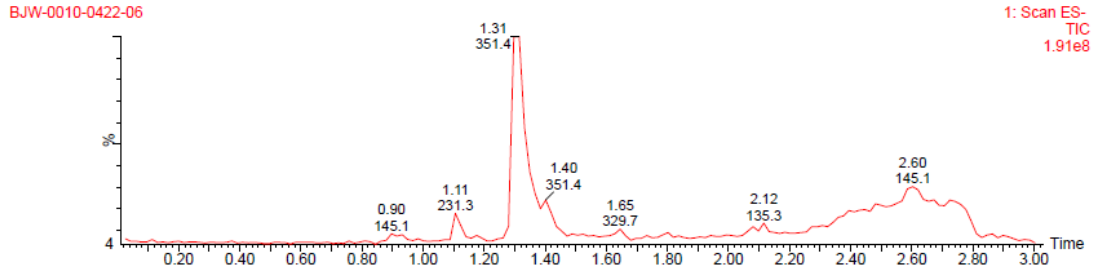
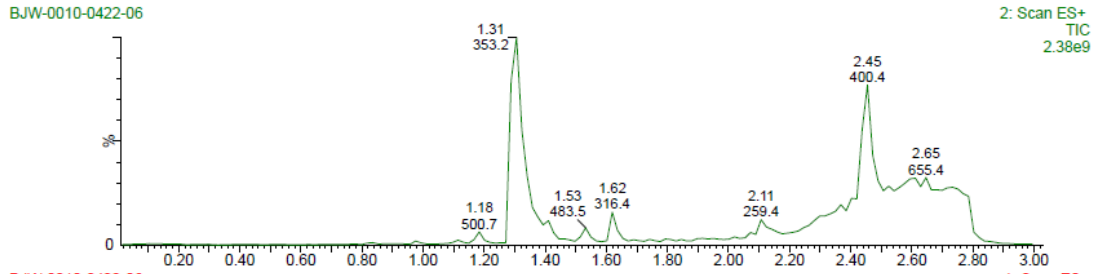
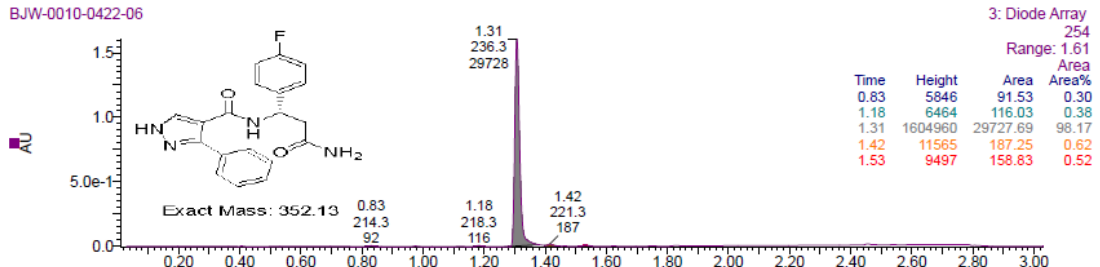


# LCMS Spectra for compound **14f**

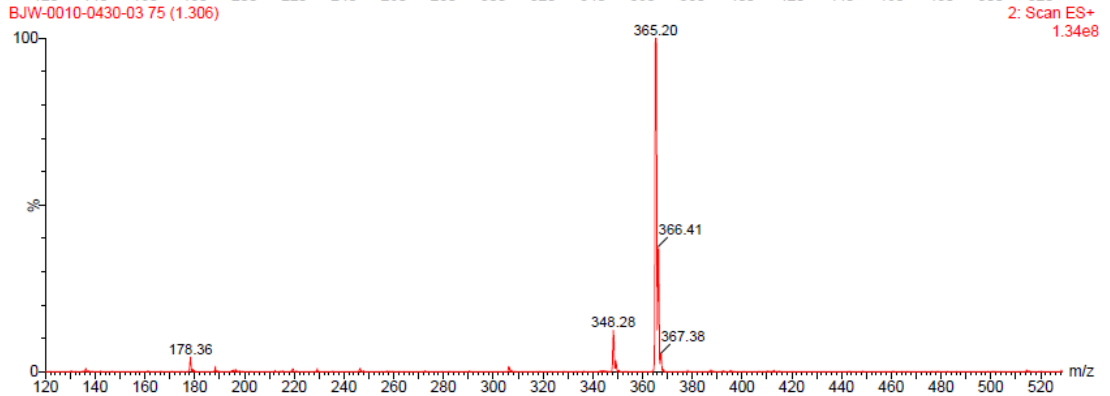
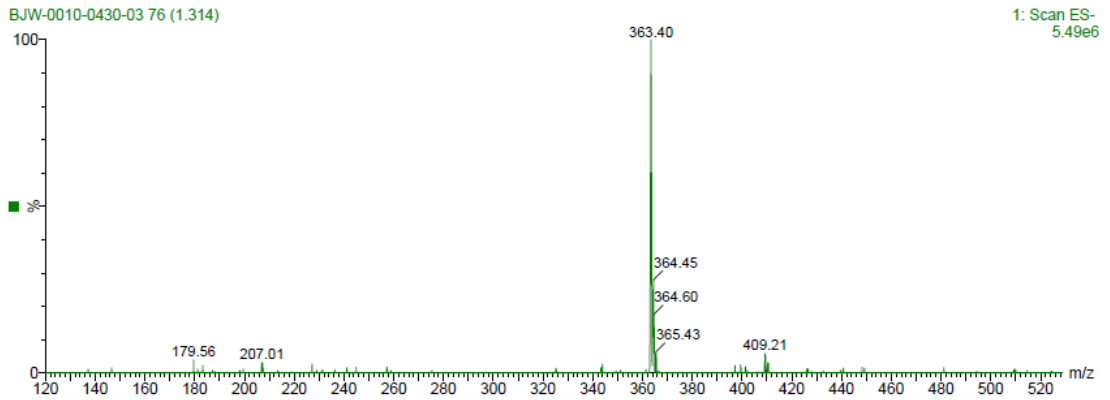
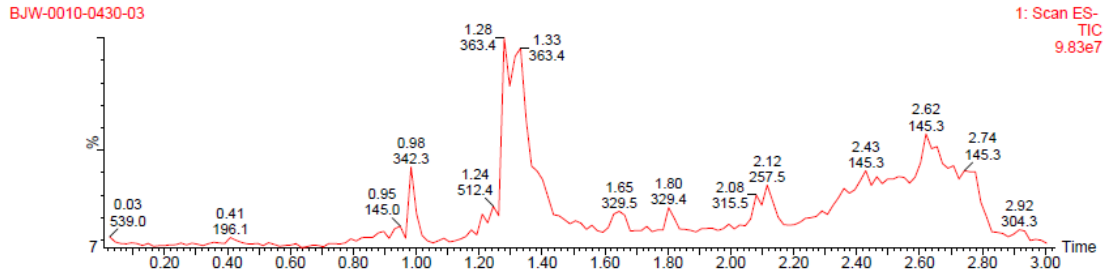
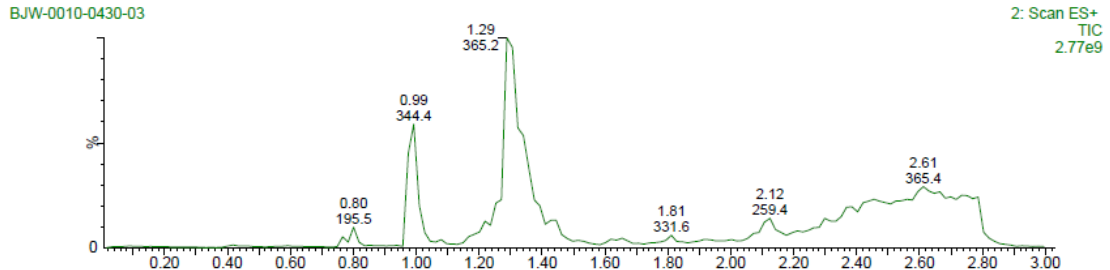
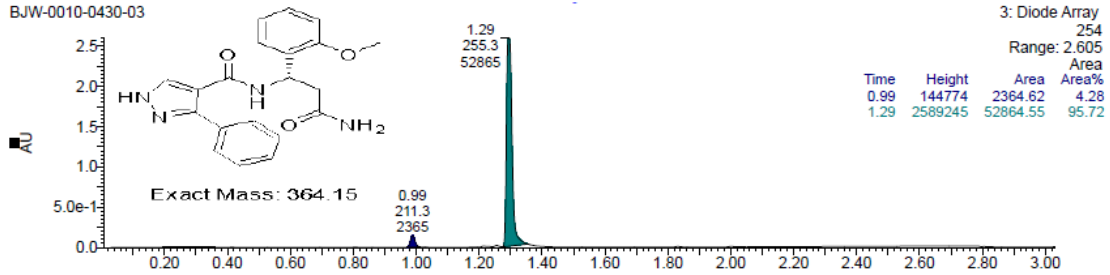




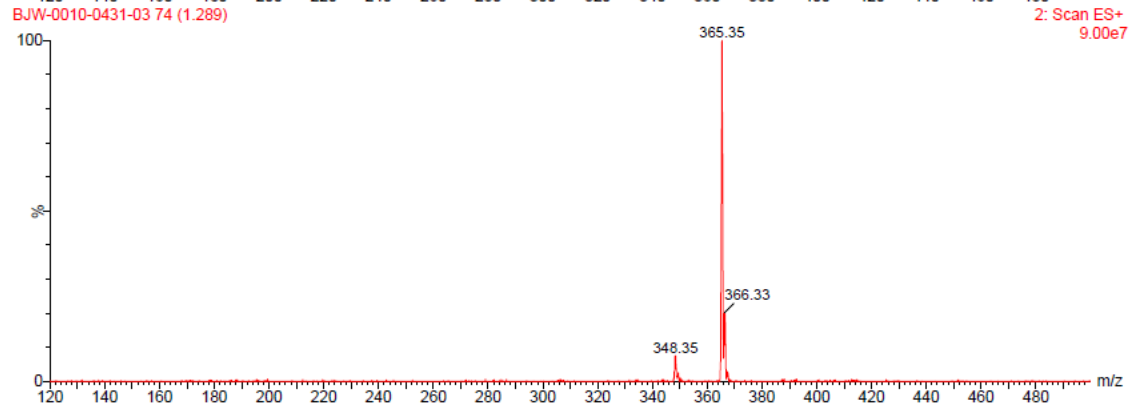
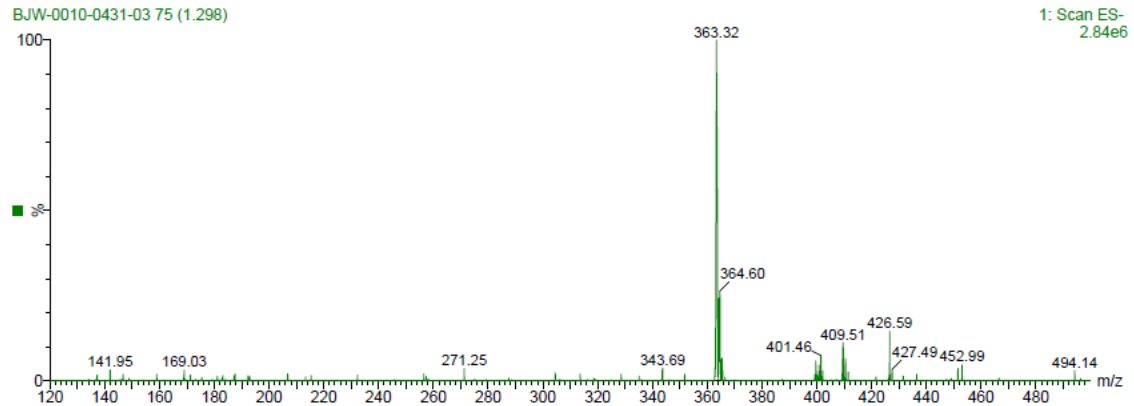
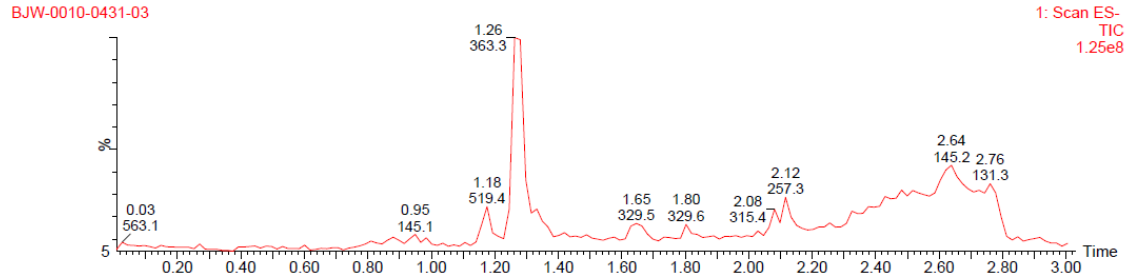
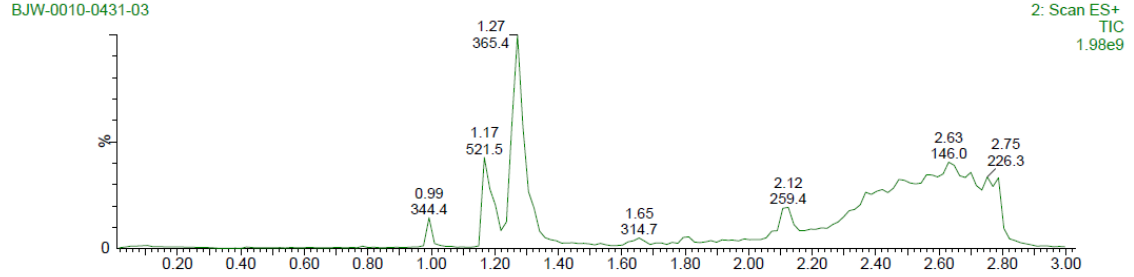
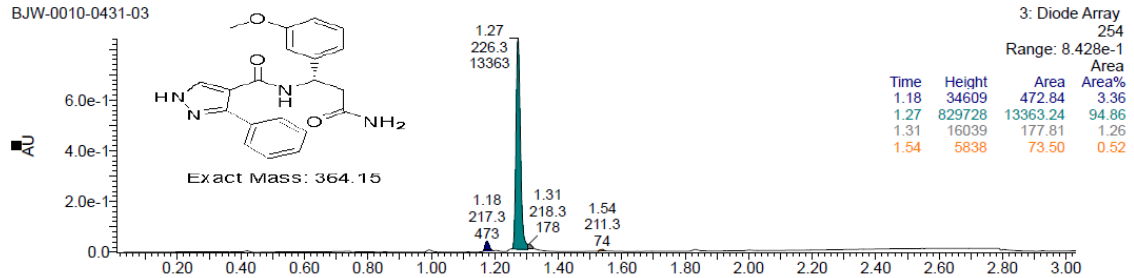
# LCMS Spectra for compound 14g



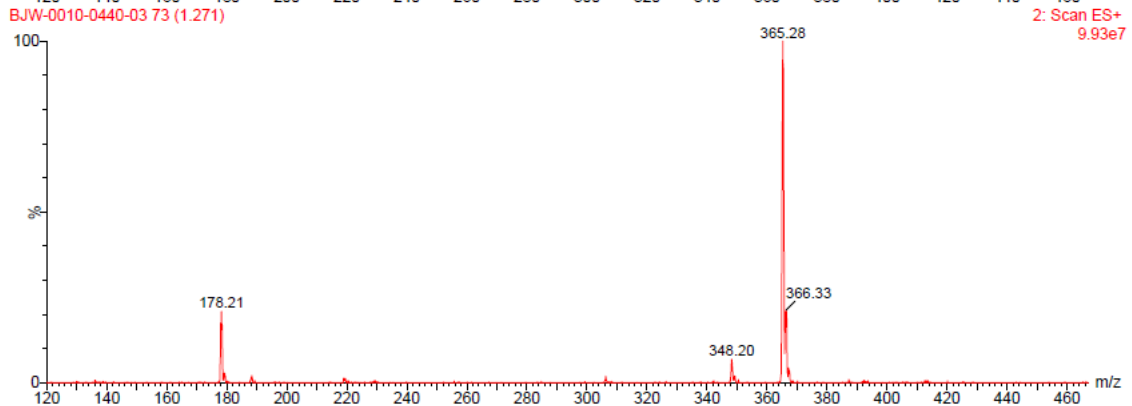
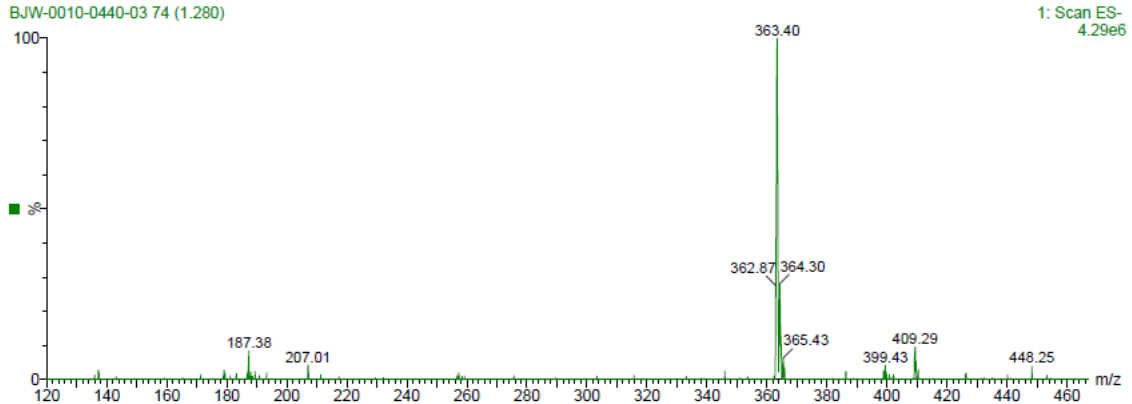
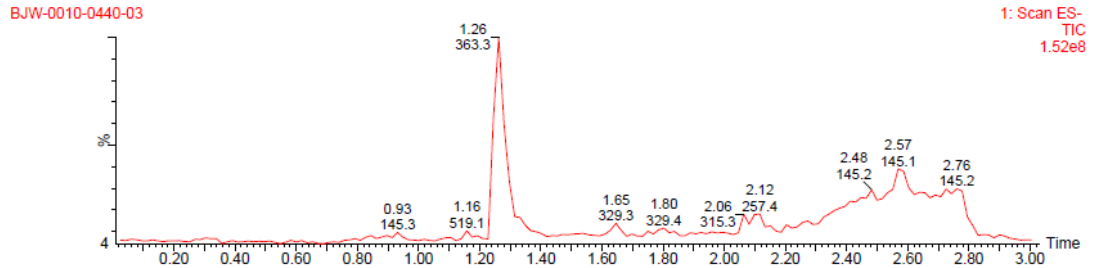
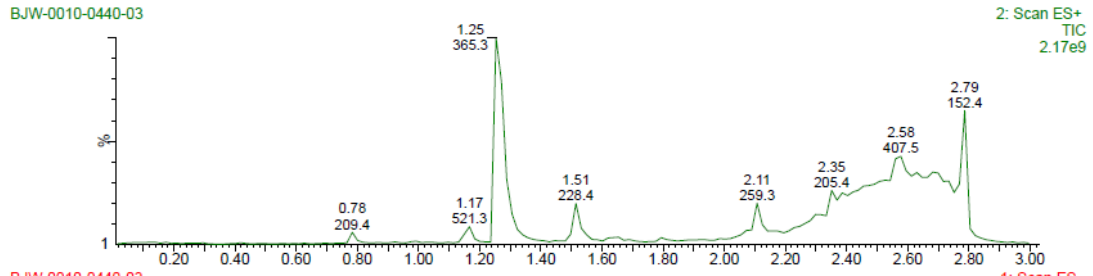
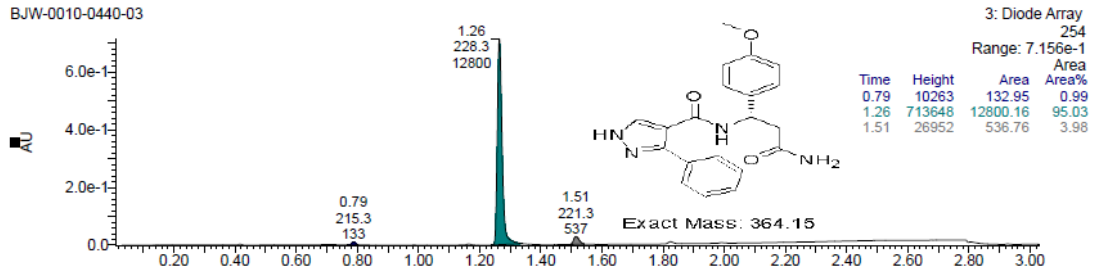
# LCMS Spectra for compound 14h



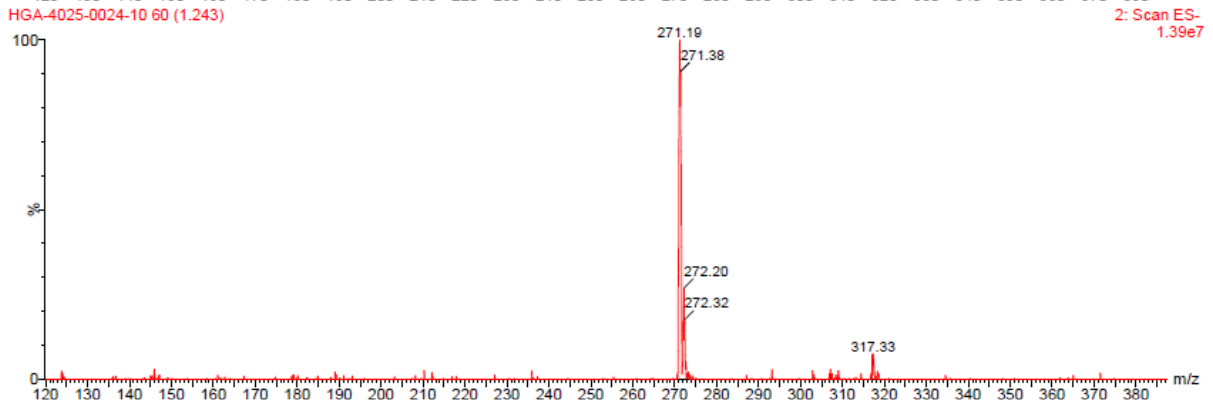
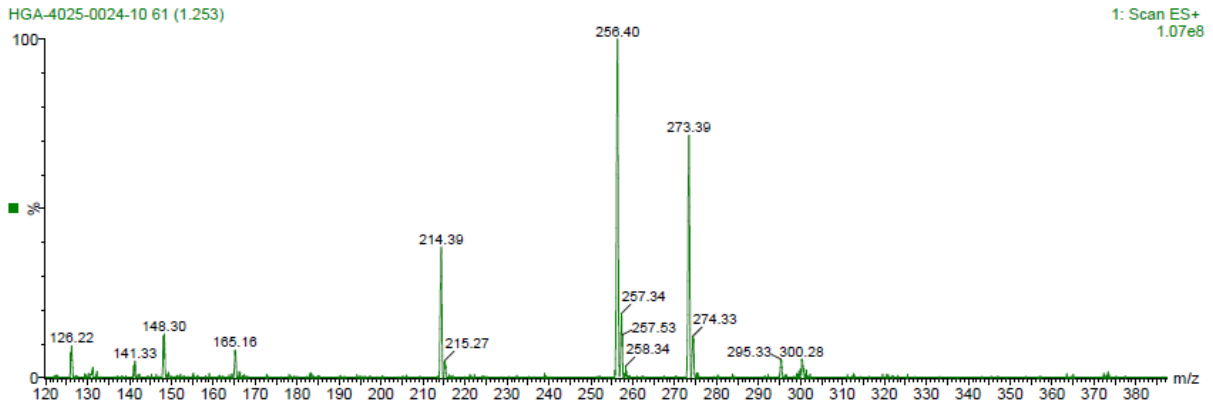
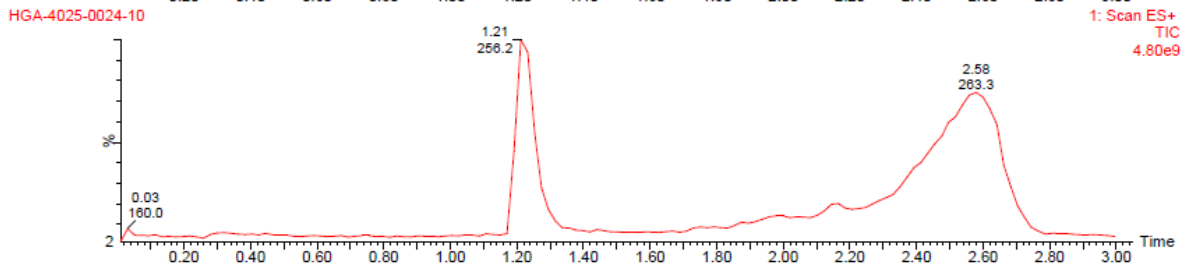
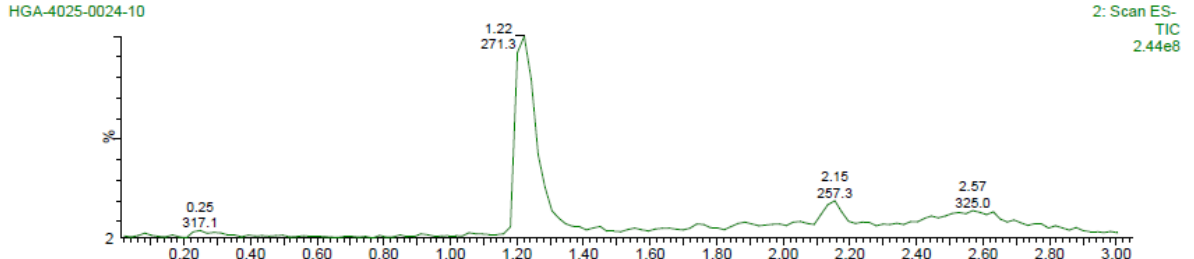
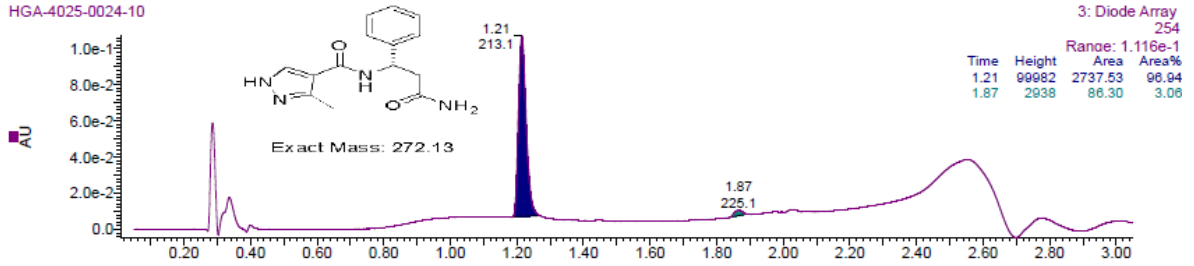
# LCMS Spectra for compound 14i



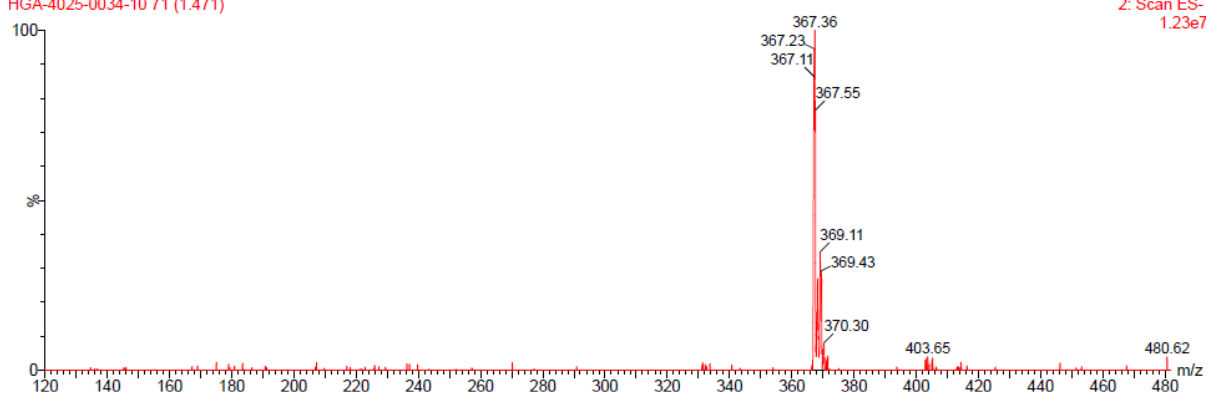
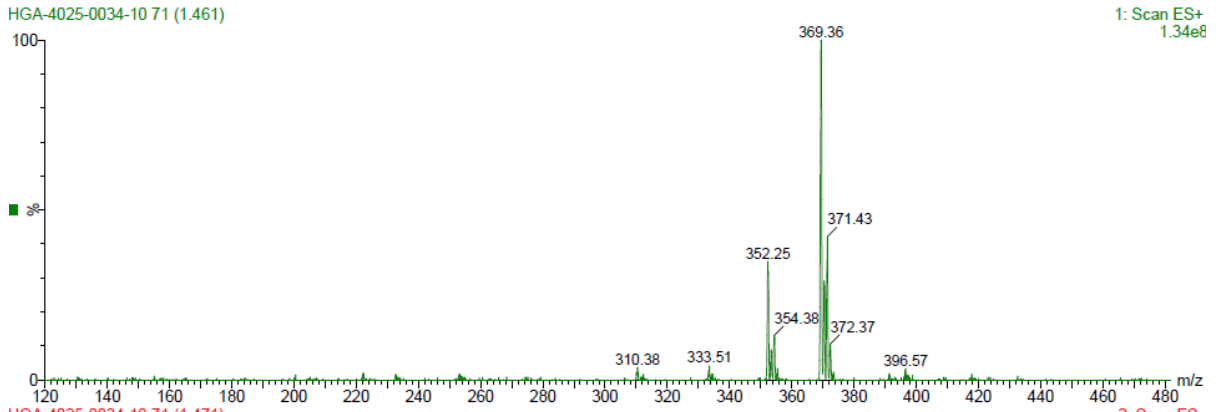
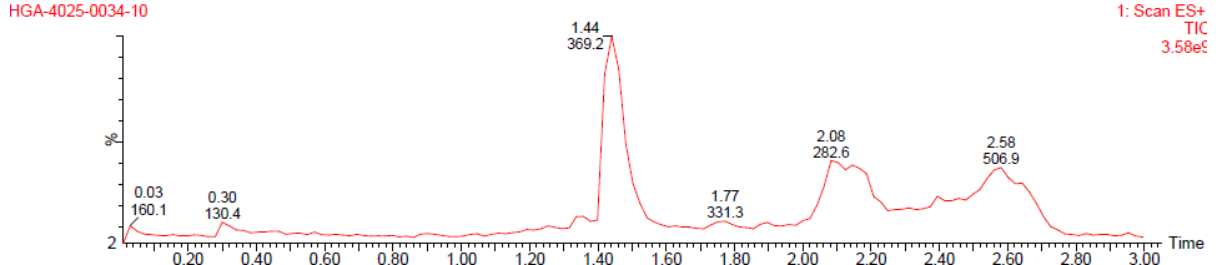
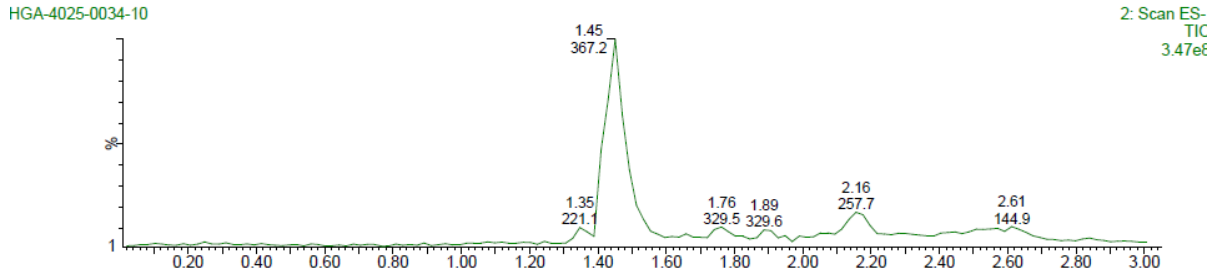
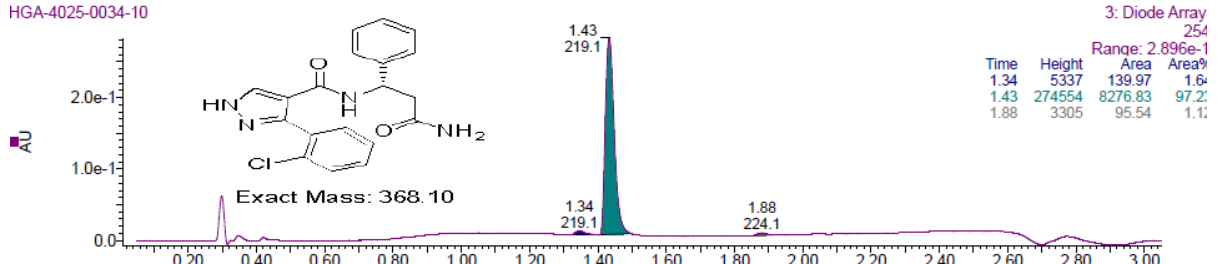
# LCMS Spectra for compound 14j



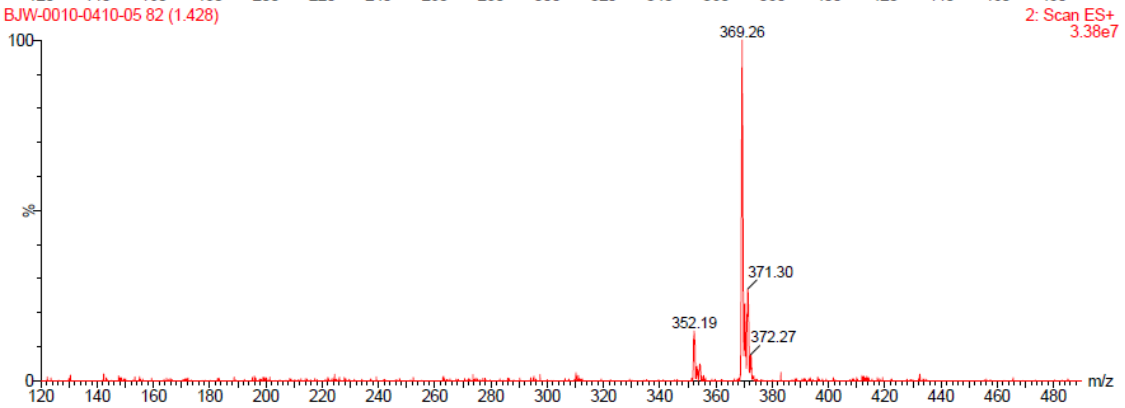
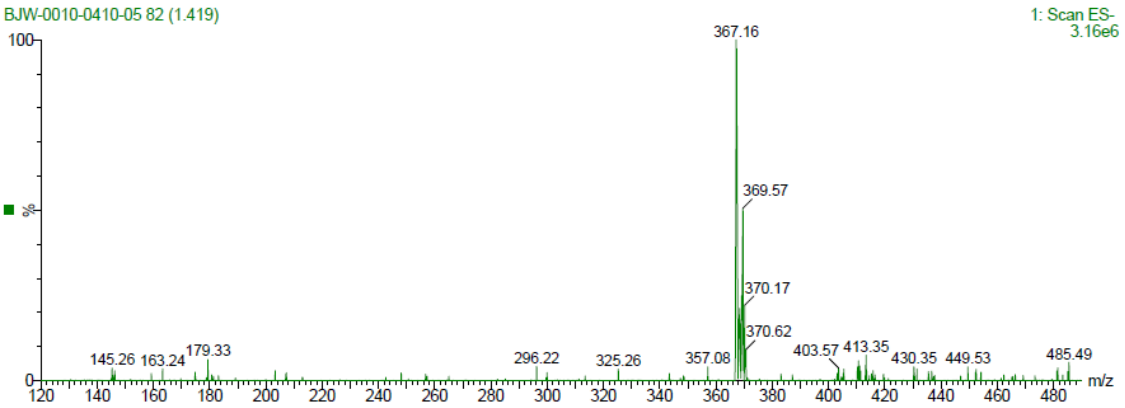
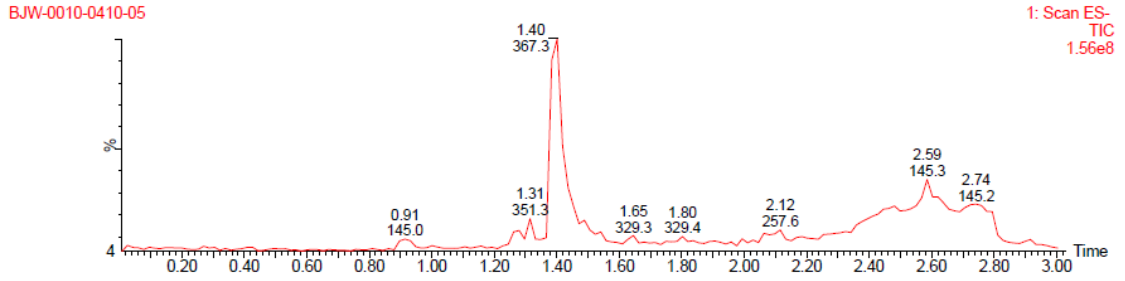
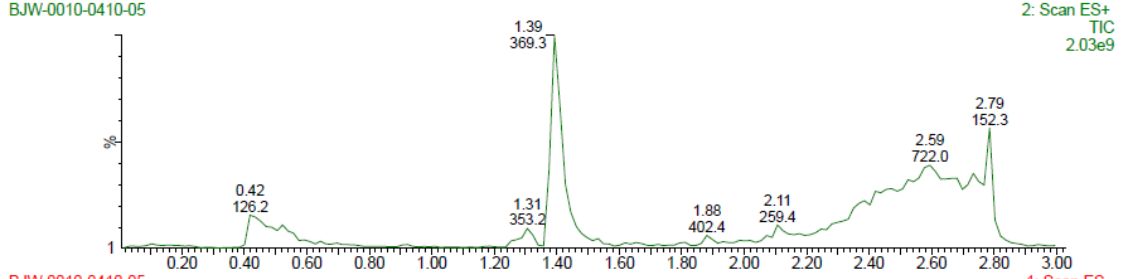
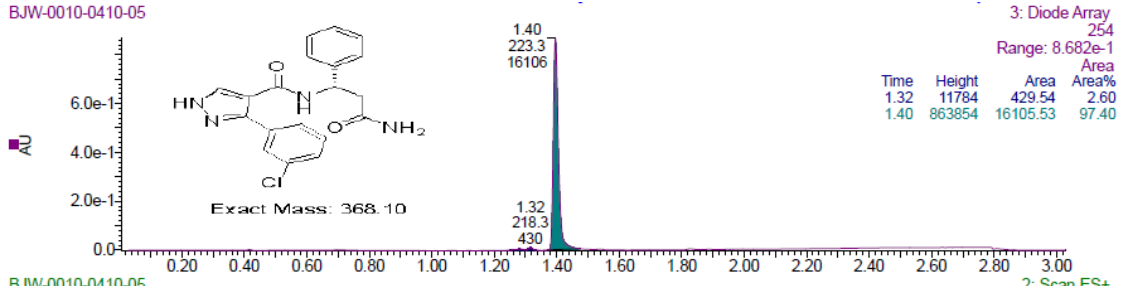
# LCMS Spectra for compound 15a



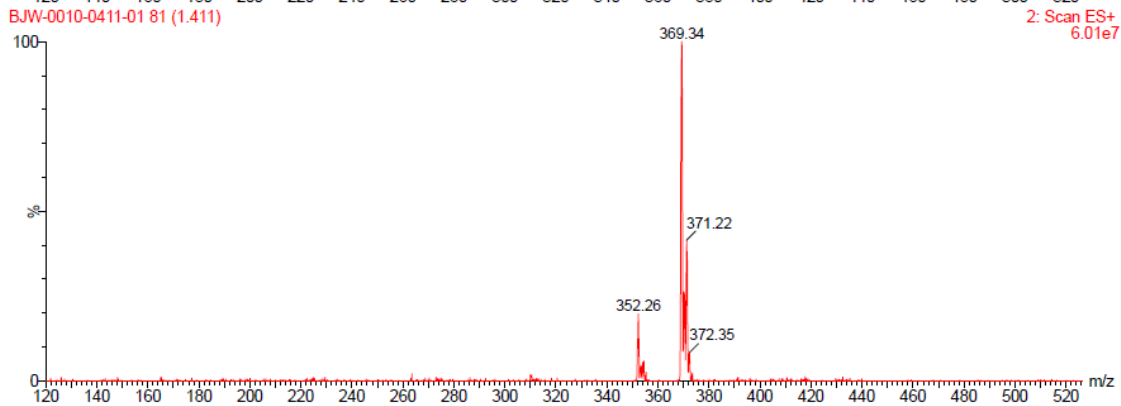
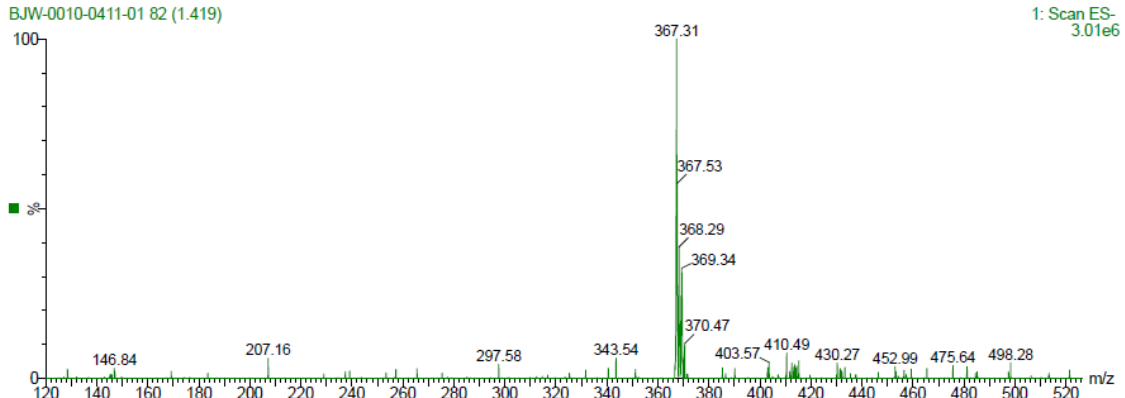
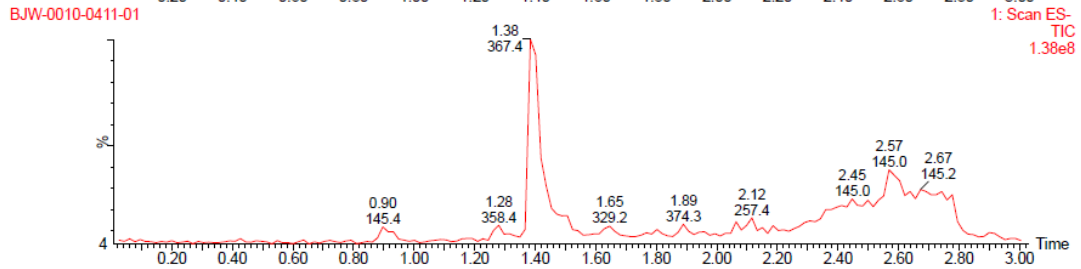
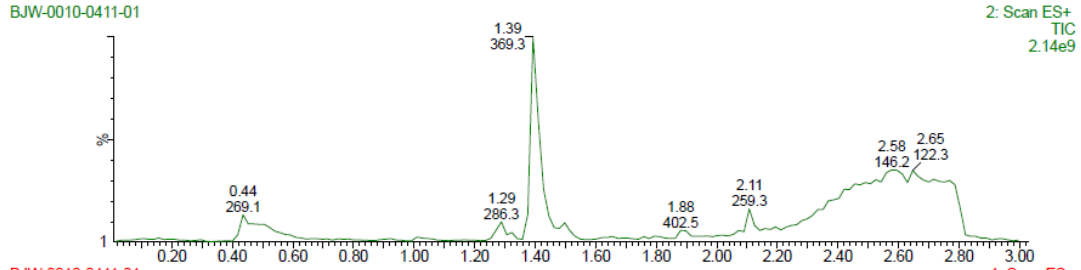
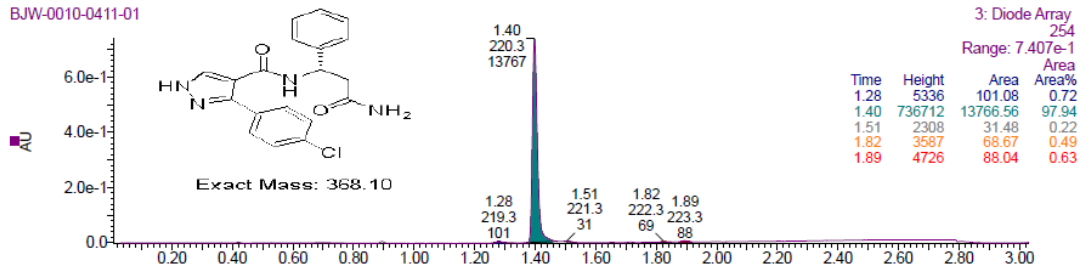
# LCMS Spectra for compound 15b



# LCMS Spectra for compound 15c

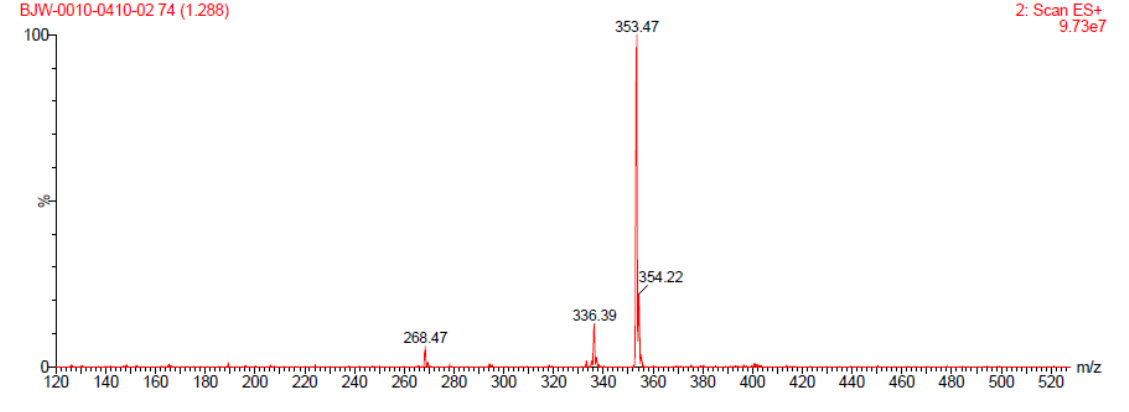
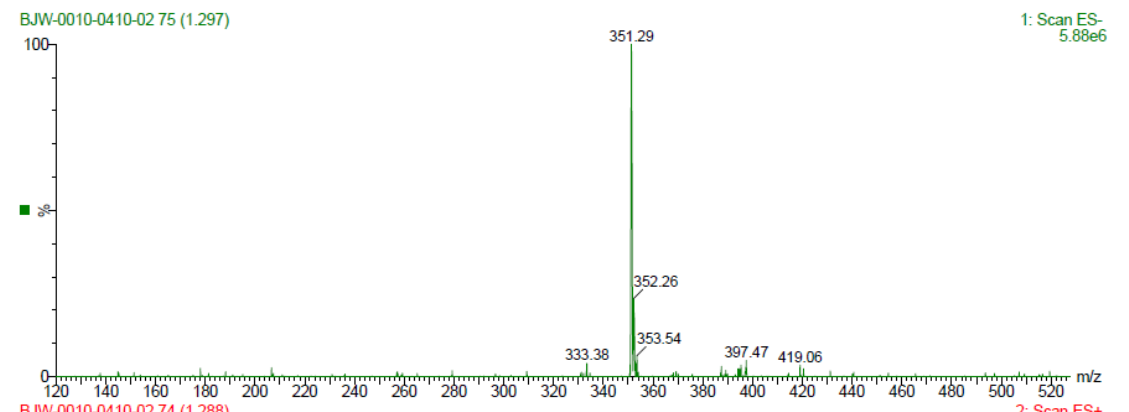
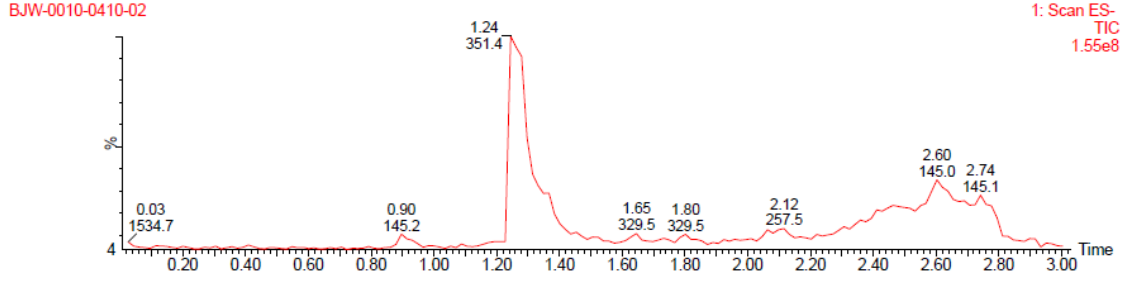
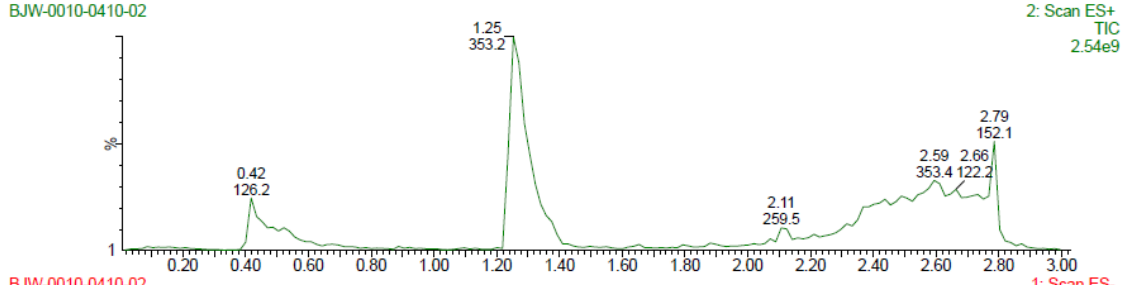
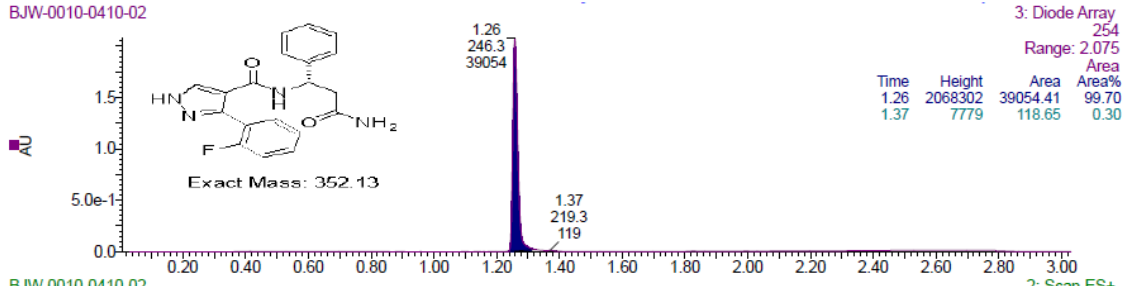


# LCMS Spectra for compound 15d

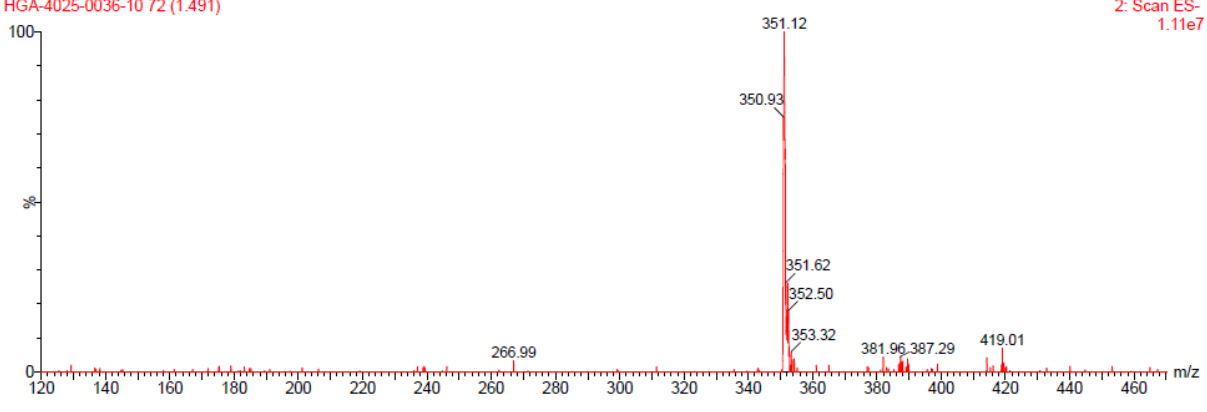
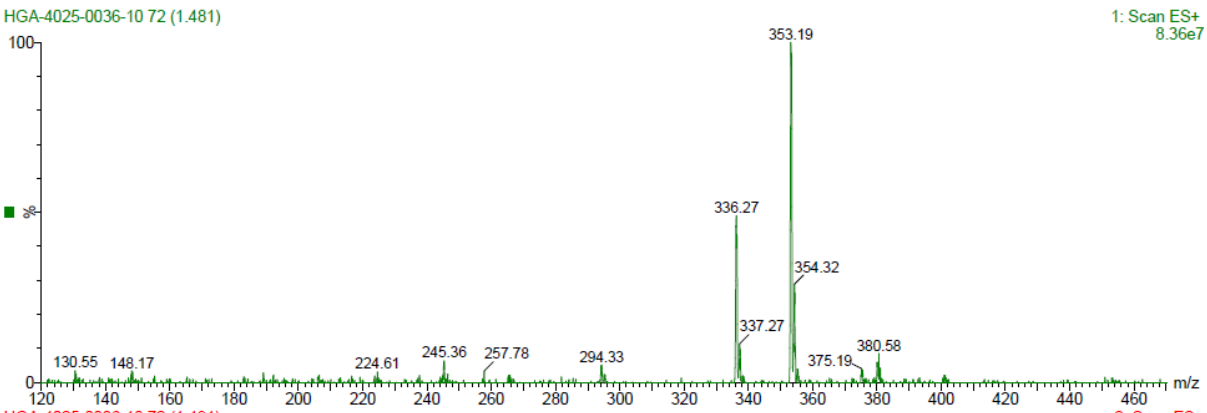
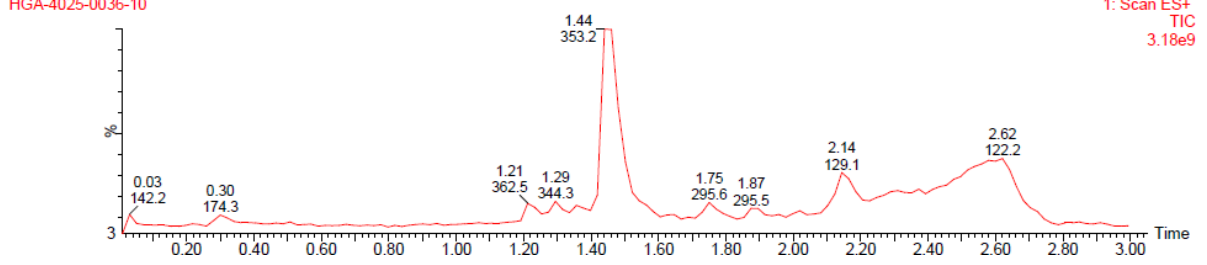
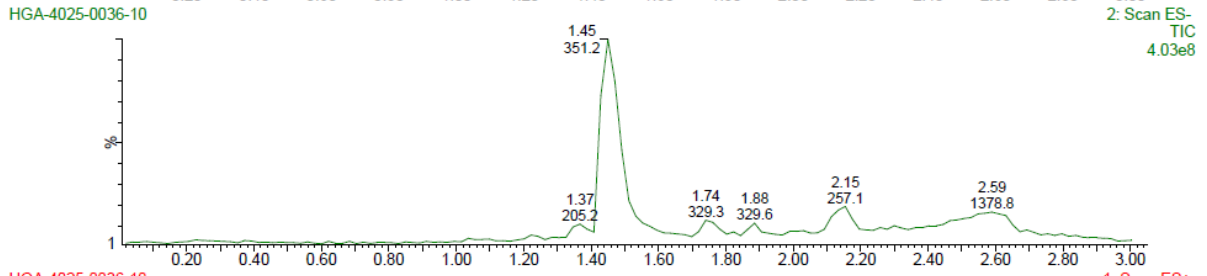
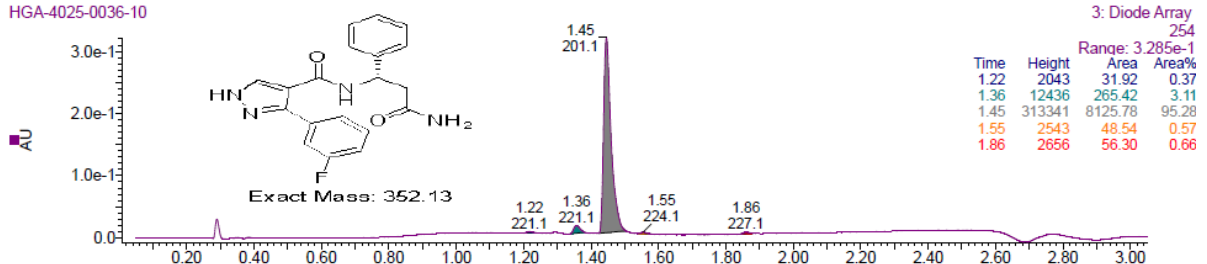




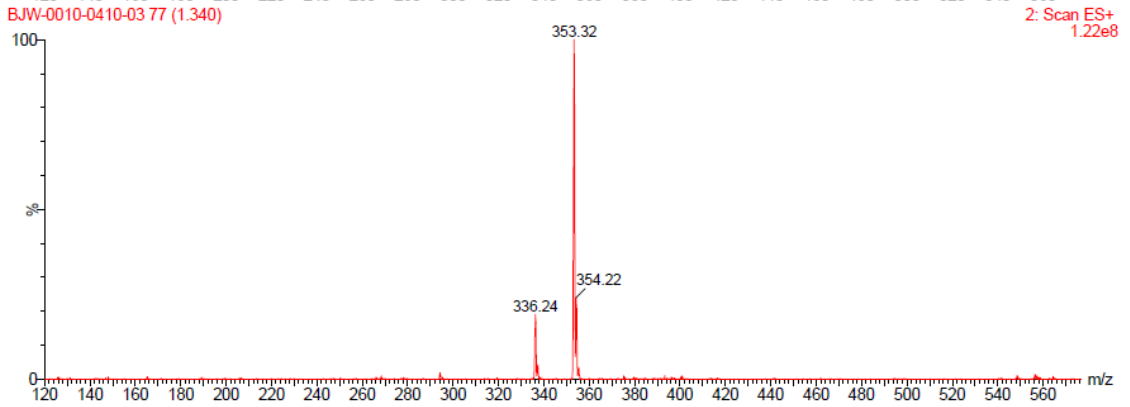
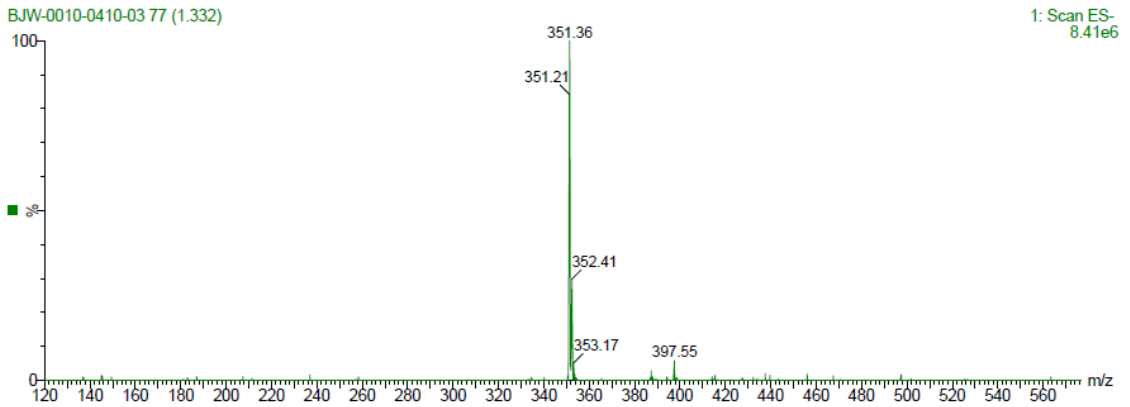
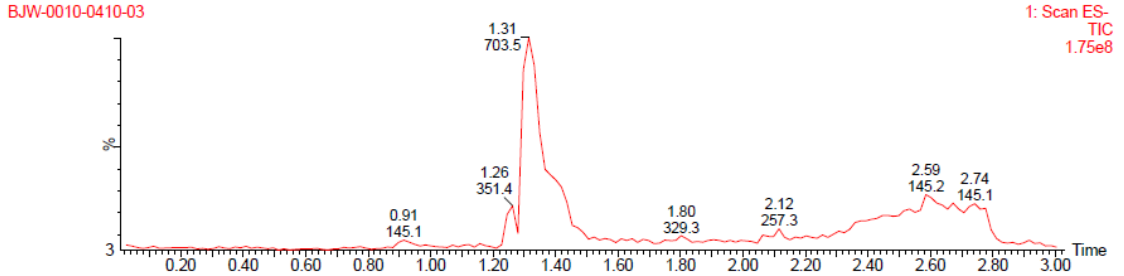
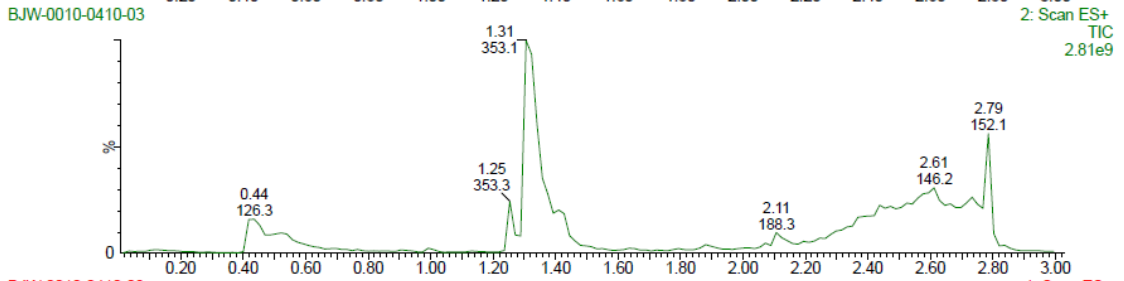
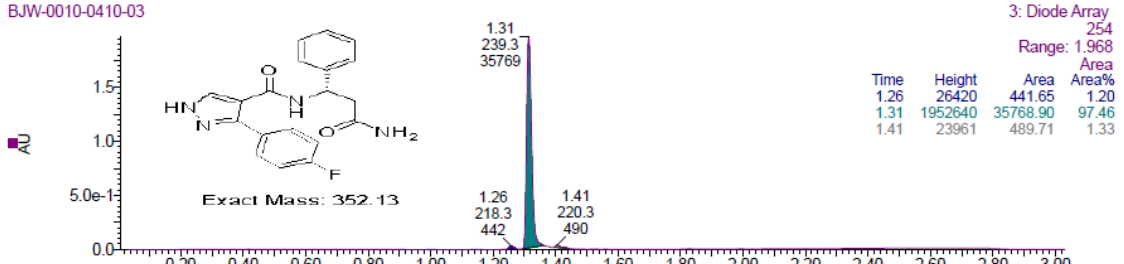
# LCMS Spectra for compound 15e



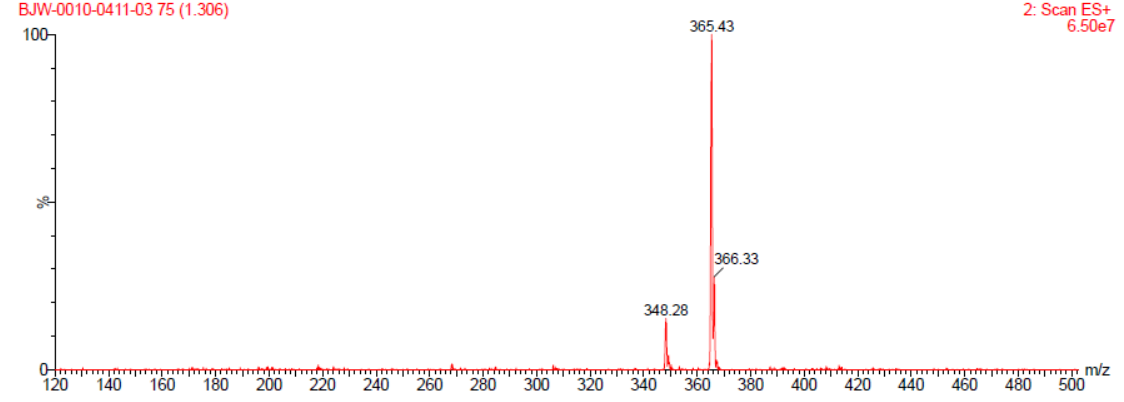
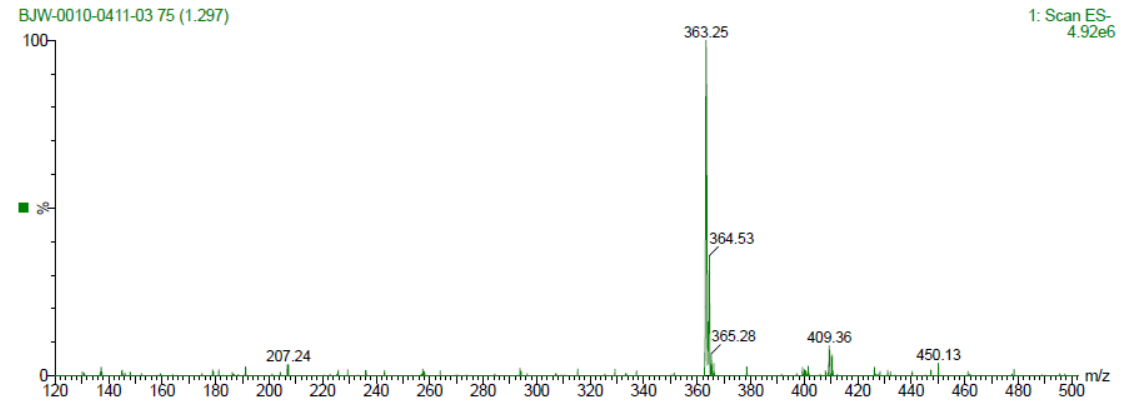
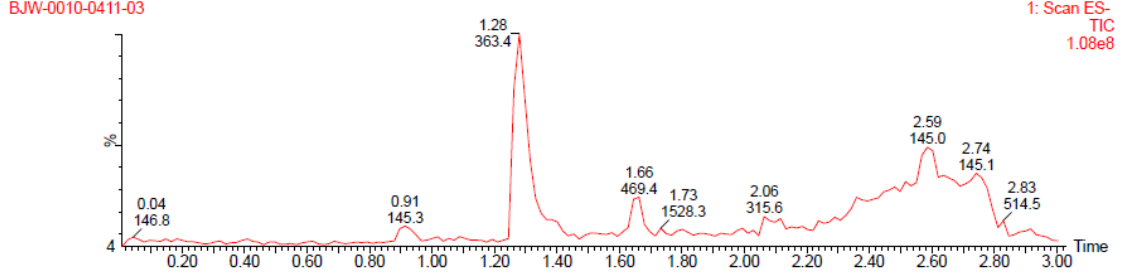
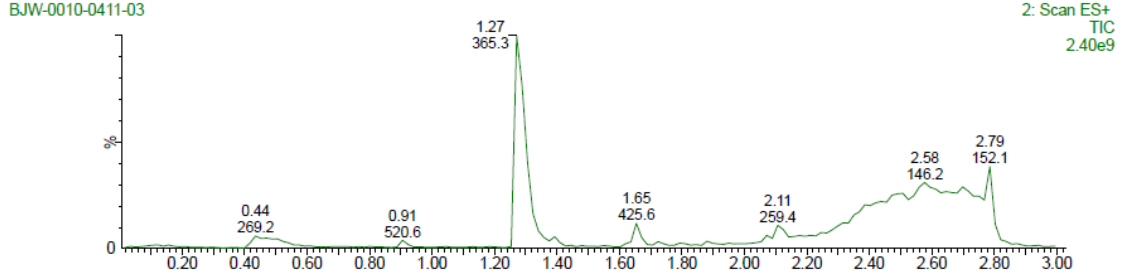
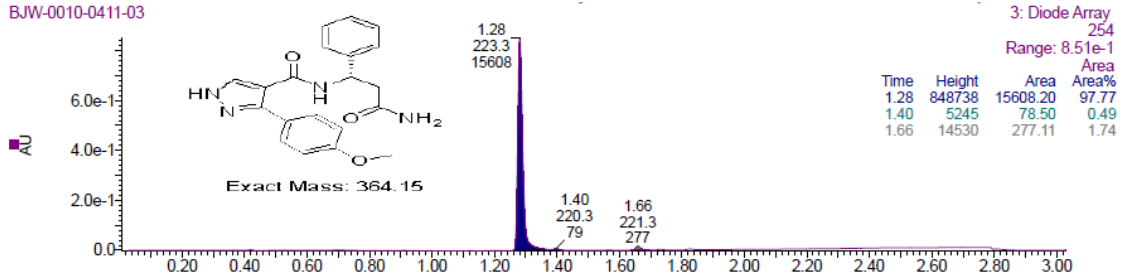
# LCMS Spectra for compound 15f



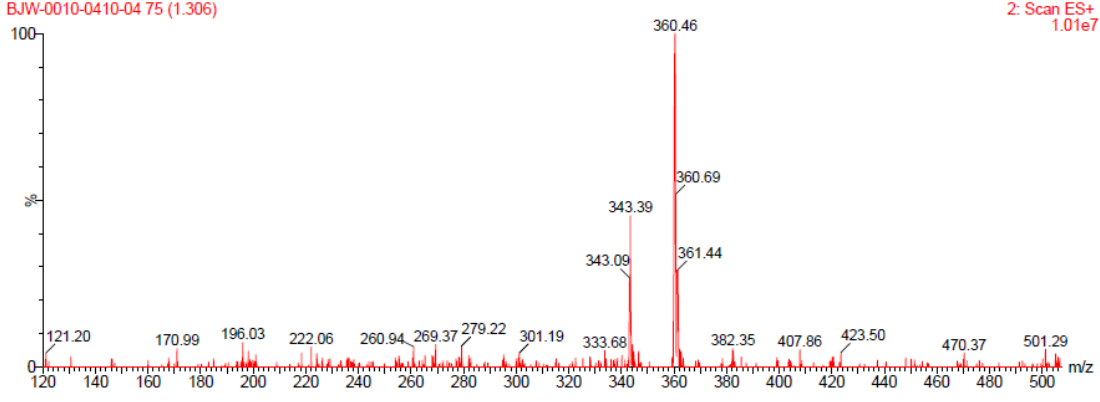
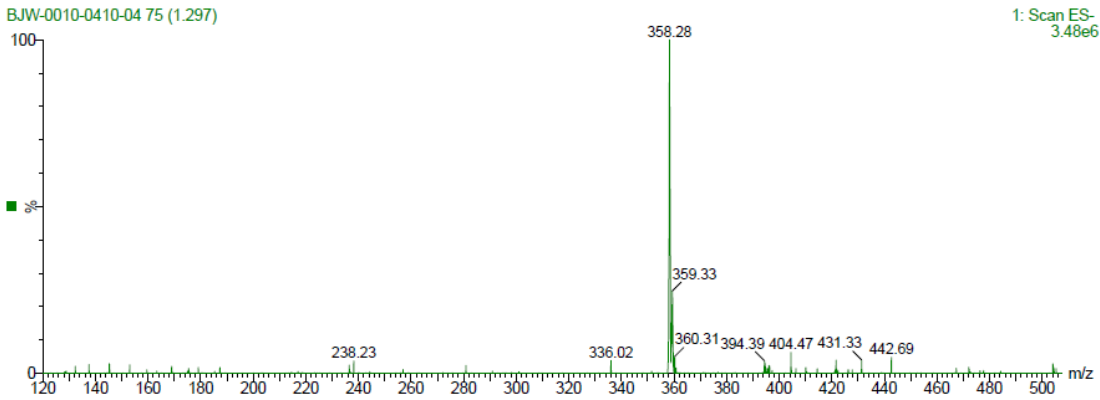
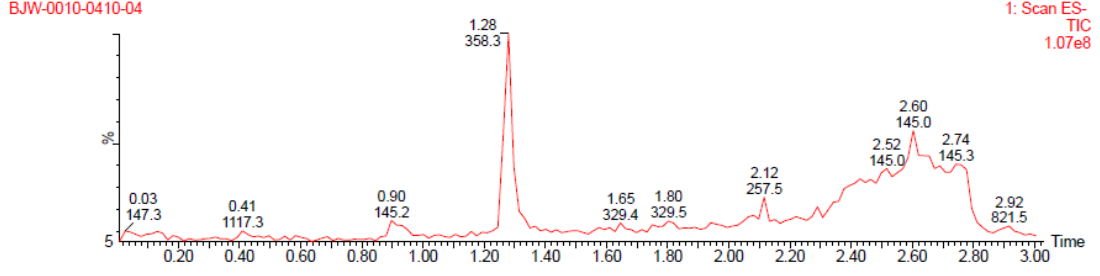
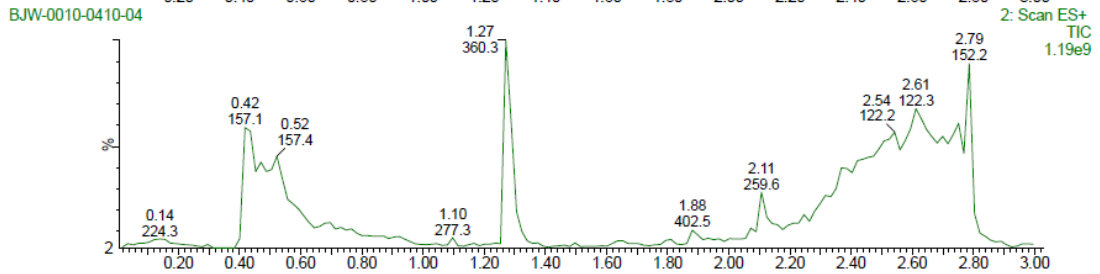
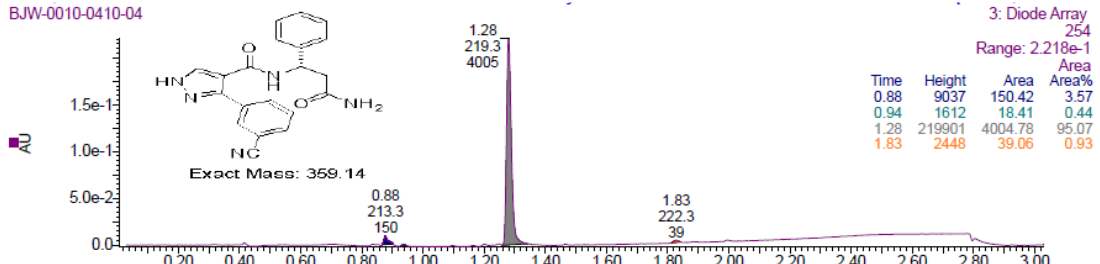
# LCMS Spectra for compound 15g



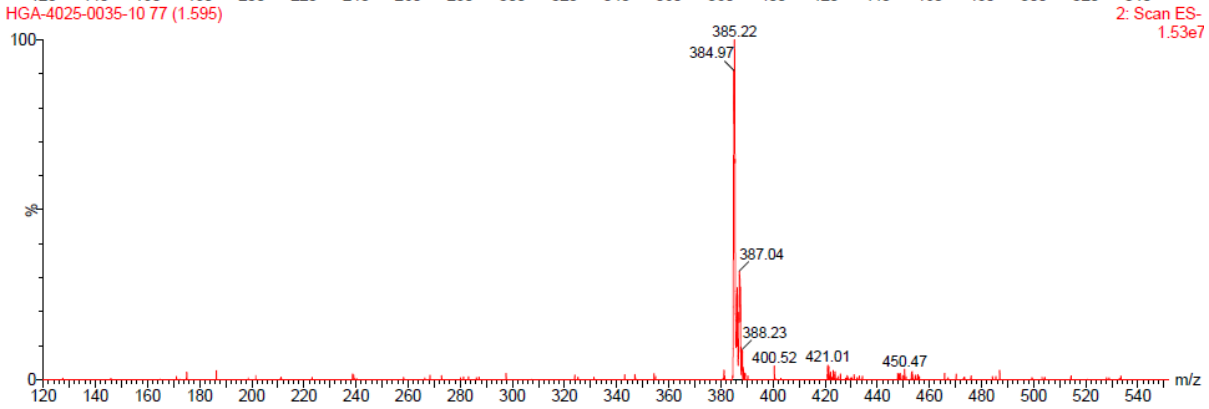
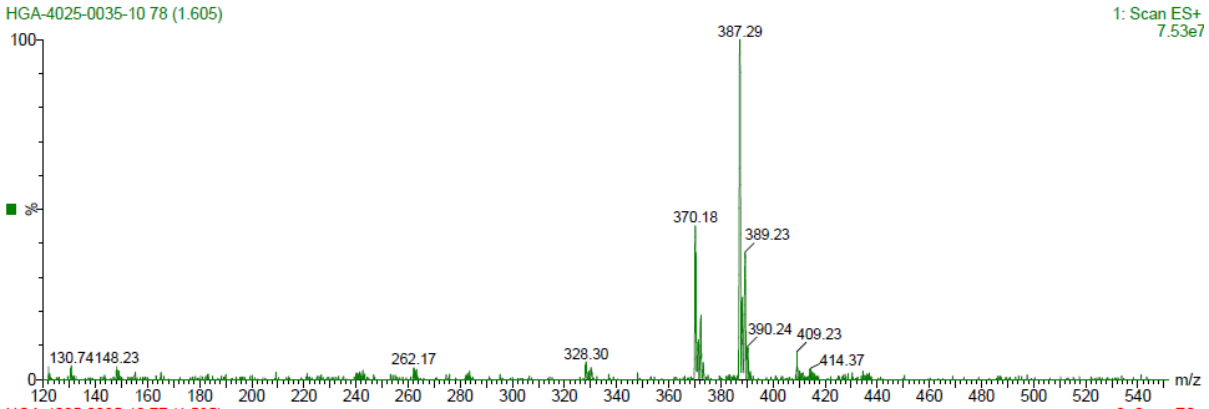
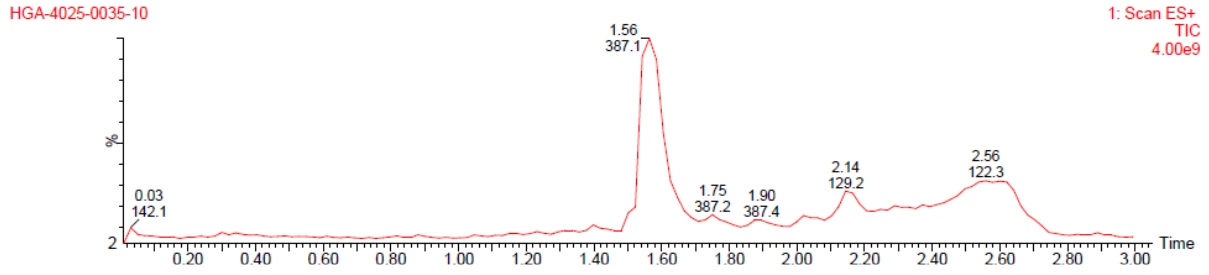
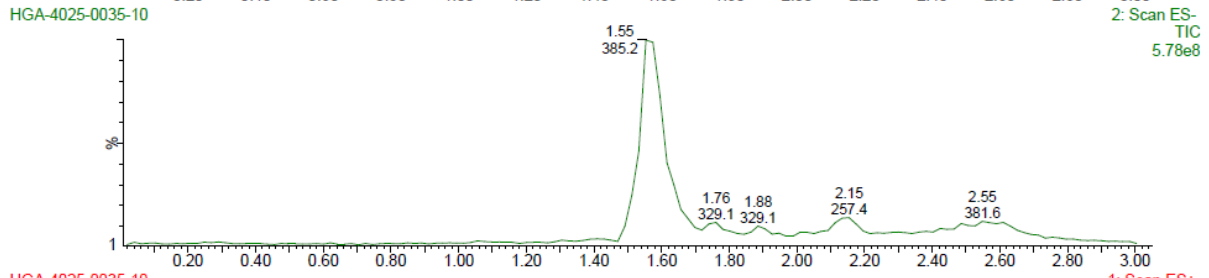
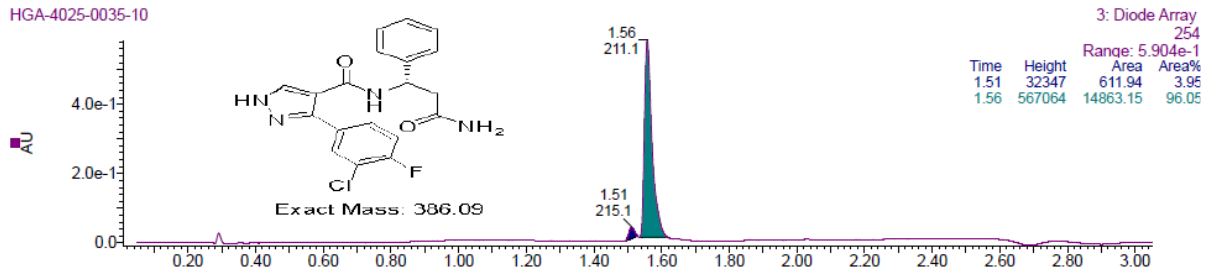
# LCMS Spectra for compound 15h



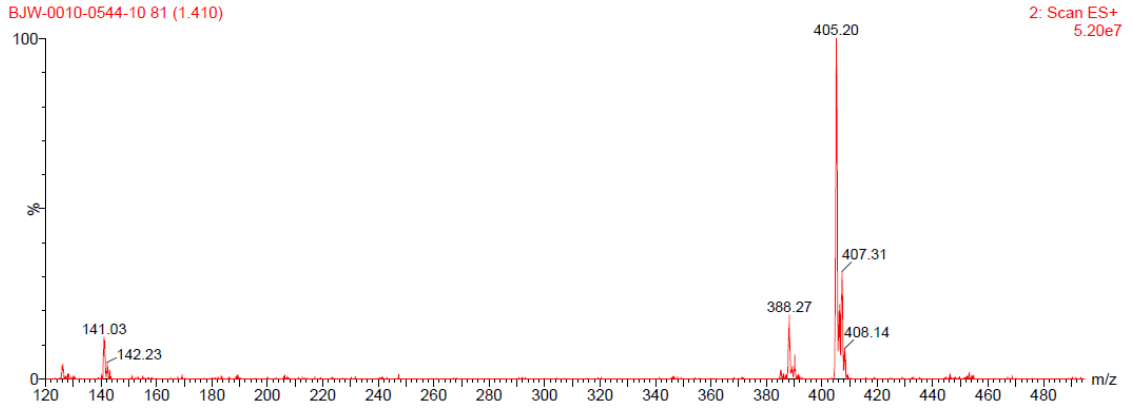
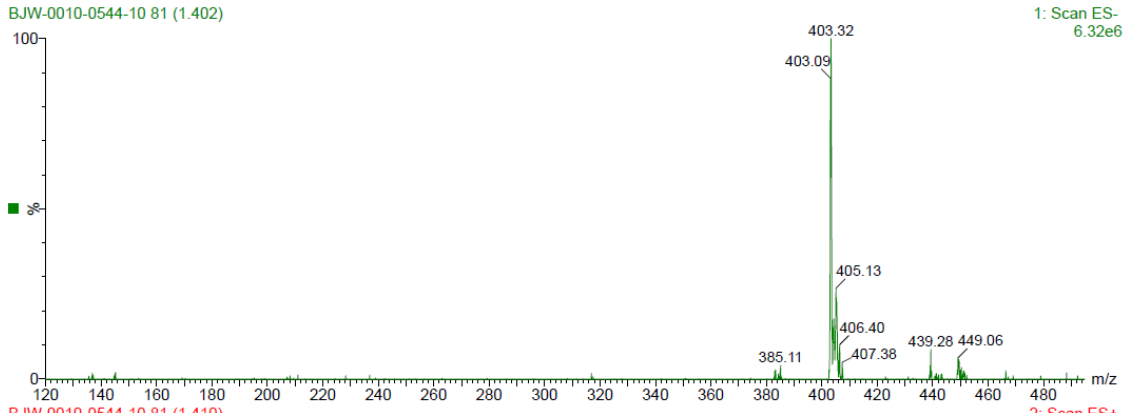
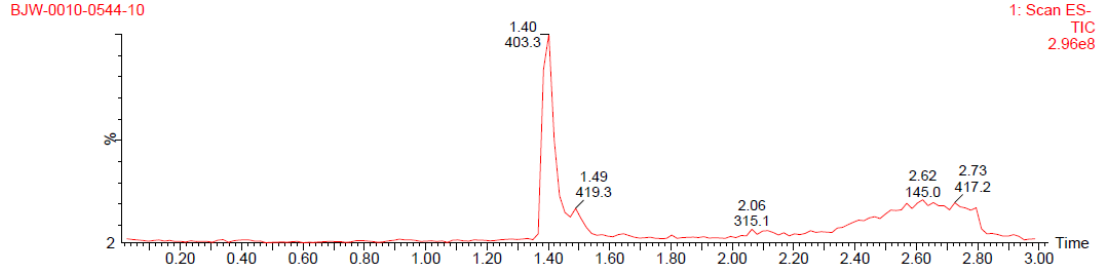
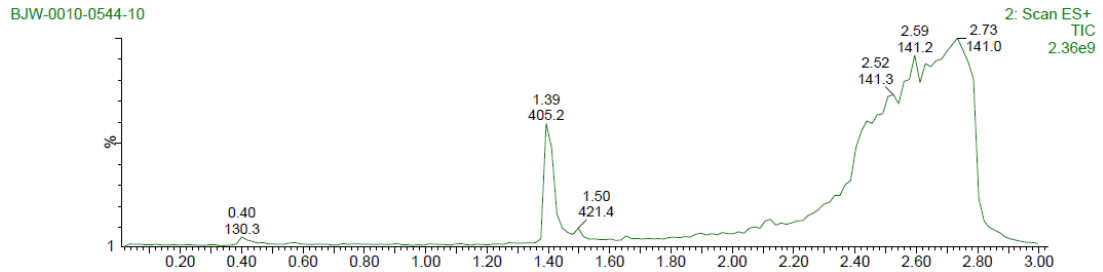
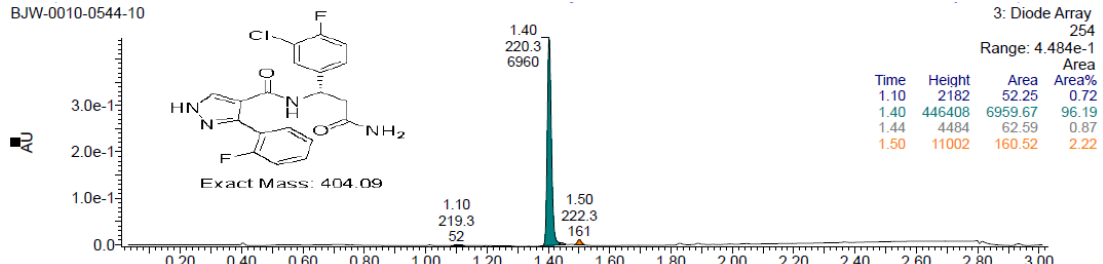
# LCMS Spectra for compound 15i



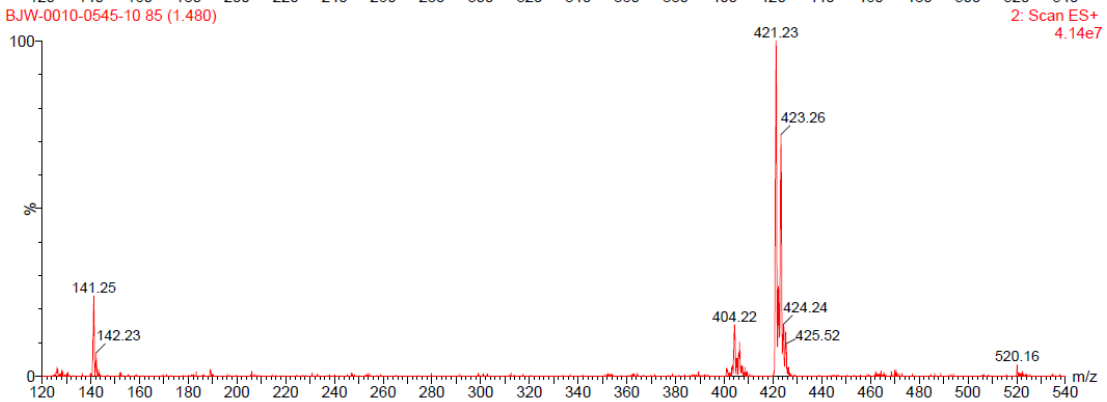
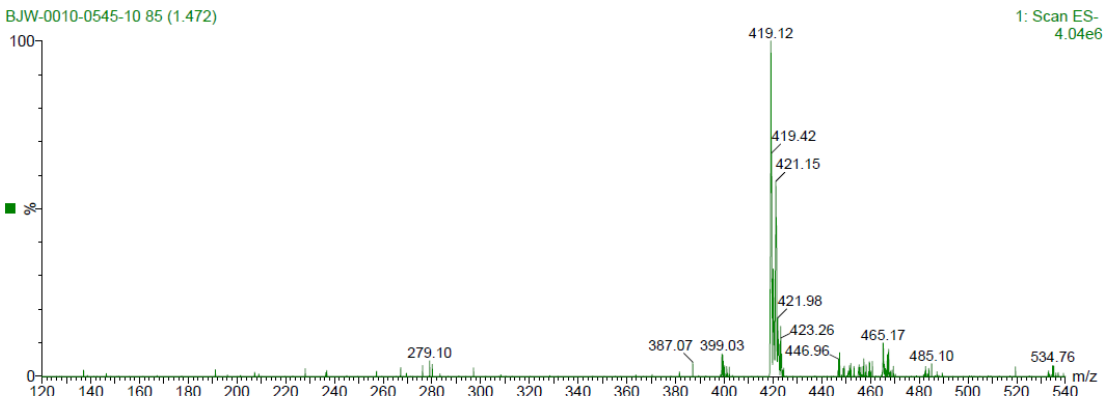
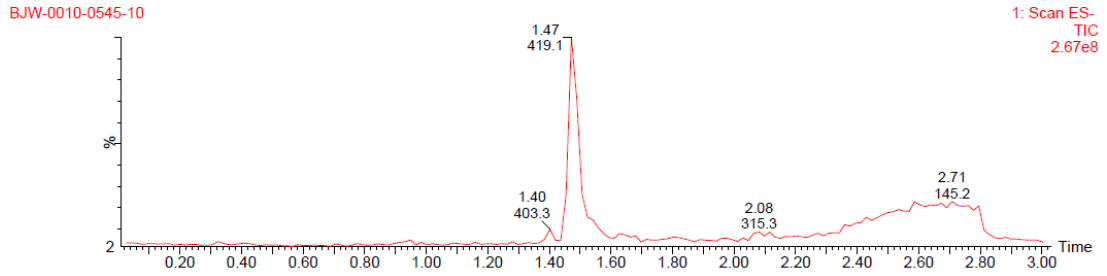
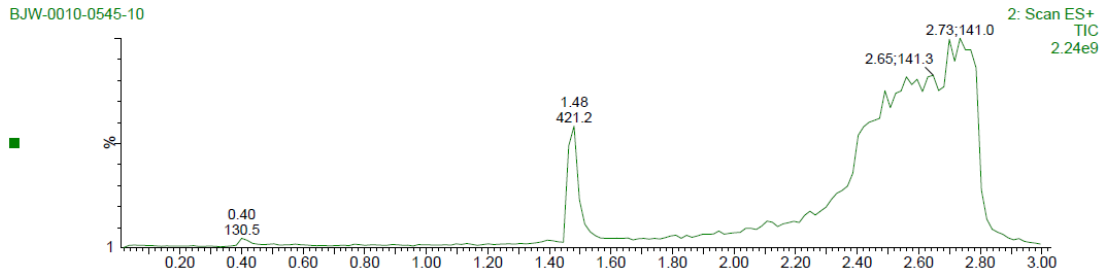
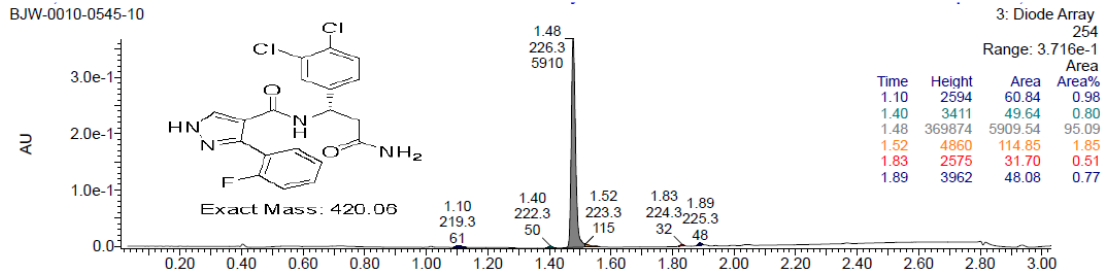
# LCMS Spectra for compound 15j



# LCMS Spectra for compound 26a

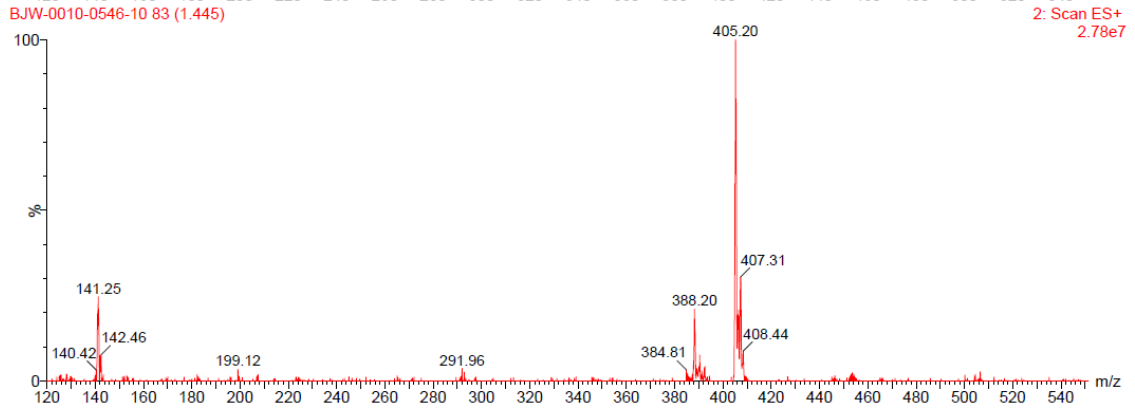
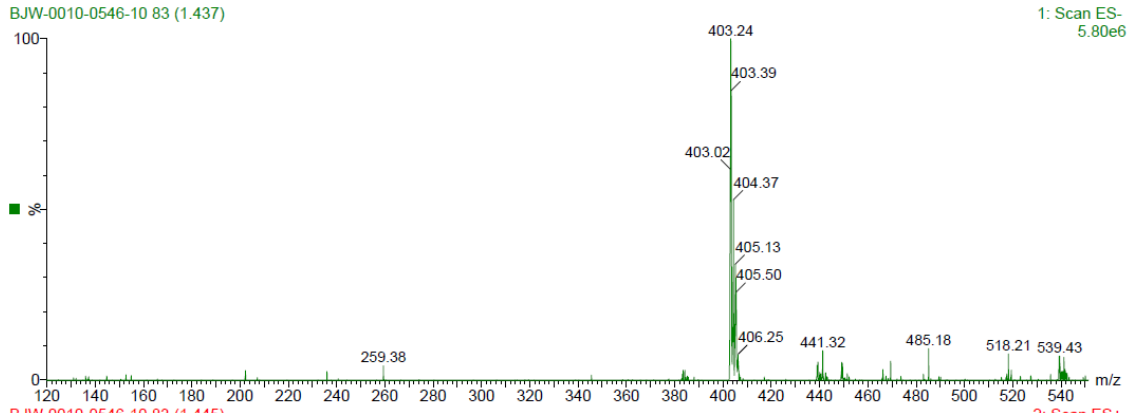
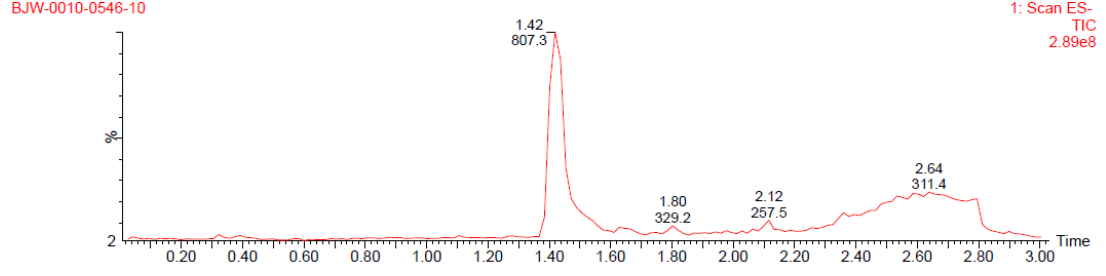
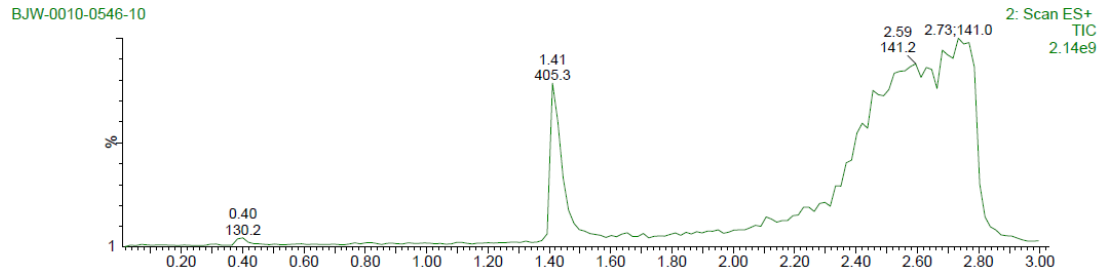
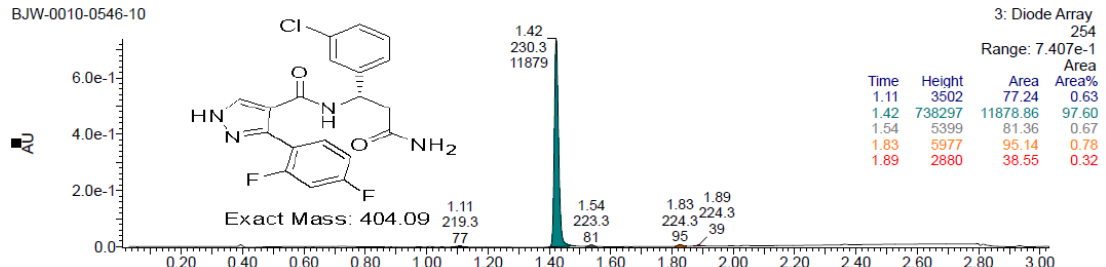


# LCMS Spectra for compound 26b

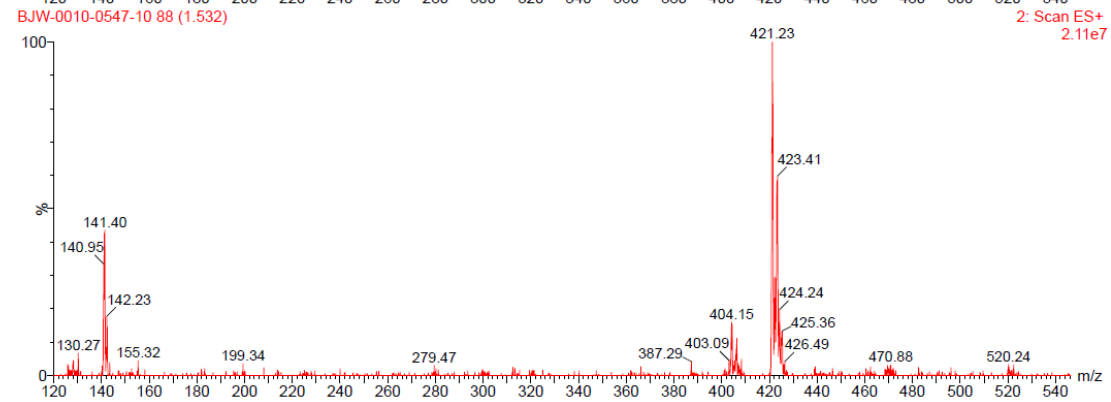
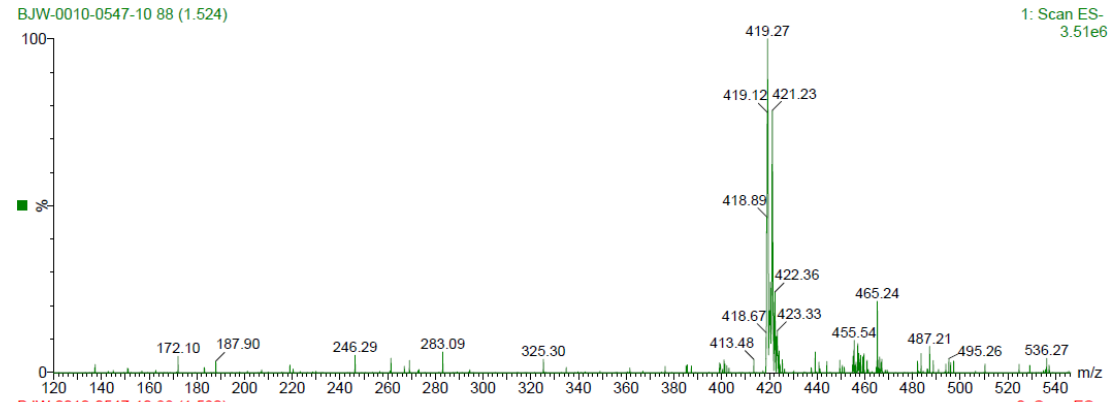
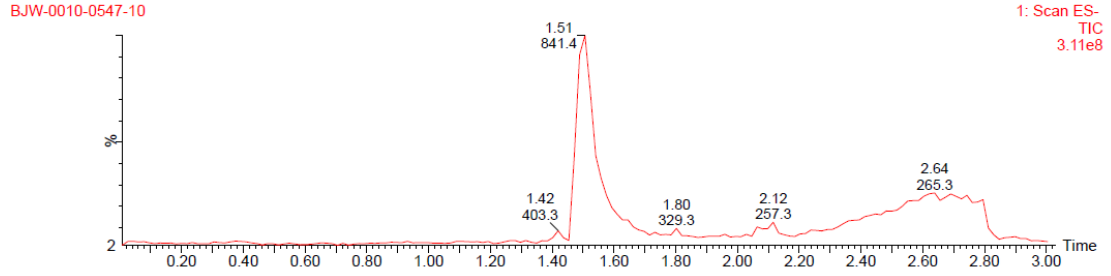
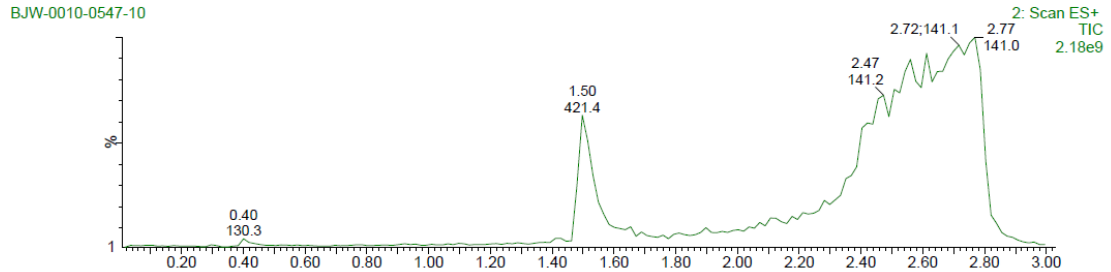
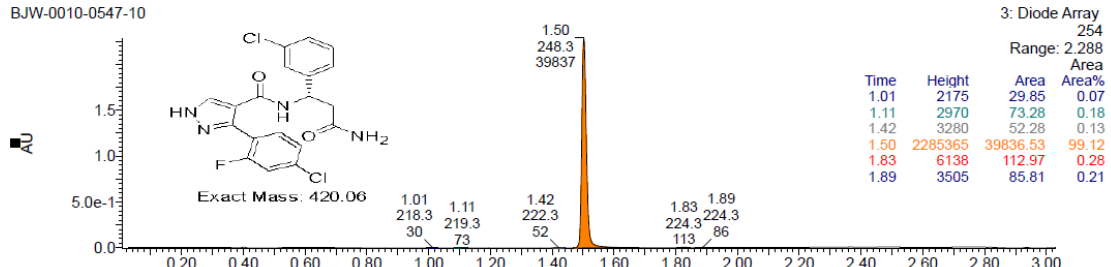




# LCMS Spectra for compound 26c



# LCMS Spectra for compound 26d



# LCMS Spectra for compound 26e

